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CONSERVATION LAWS AND FERN-EQUIVALENCE IN GENERAL RELATIVITY

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(Received January 24, 1961)

A generalized parallelism (called fern-equivalence), fern-equivalent tetrads, and quasi-cartesian coordinates are defined in riemannian geometry with the help of one-parametric families of extremal (minimal) hypersurfaces. The same ideas are applied to secure conservation laws and localization of energy, momentum, and angular momentum in general relativity.

1. Introduction

In a paper entitled "*Riemann-Geometrie mit Aufrechterhaltung des Begriffes des Fernparallelismus*" by Einstein (1928) there was expressed the following opinion: „*Die Riemannsche Geometrie ist dadurch charakterisiert, dass... die Beträge zweier Linienelemente, welche den infinitesimalen Umgebungen zweier endlich voneinander entfernter Punkte P und Q angehören, miteinander vergleichbar sind. Dagegen fehlt der Begriff der Parallelität solcher zweier Linienelemente; der Richtungs-begriff existiert nicht für das Endliche*“.

This opinion, or rather its second part, shared generally by physicists, is based upon the fact that, according to the well known definition of parallel displacement, the result of the parallel displacement is not unique but depends upon the path of the displacement. In particular, a vector displaced parallelly from the point P along a closed path back to the same point is no more the same vector. However, the above quoted opinion is misleading. Einstein himself denies it in the same article by looking for a definition of fern-parallelism.

Led by his physical intuition, Einstein regarded the lack of the concept of fern-parallelism as a serious drawback hampering the physical interpretation and tried to supplement the riemannian geometry by a prescription permitting to decide which one of the variety of directions at a point Q is to be regarded as "parallel" to a given direction at the point P .

To achieve this end he introduced a tetrad field h_a^λ (greek indices or numerals 1,...4 denote components while latin indices from the beginning of the alphabet or numerals in parenthesis (1),...(4) denote vectors constituting the tetrad). Then he defined in terms of h_a^λ some analogue of the affine connection permitting to formulate a unitary theory of

gravitation and electromagnetism. Which of the directions at Q is to be called fern-parallel to a given direction at P , depends — according to Einstein — upon the actual state of the gravitational and the electromagnetic fields.

One of the aims of the present paper is to show that, besides the einsteinian concept of fern-parallelism, there exists another, by far simpler alternative. It is possible to generalize the notion of parallelism in such a straightforward and natural way that (not only line elements but also) directions at any two points become comparable within the framework of riemannian geometry.

In order to distinguish our concept of fern-parallelism from that of Einstein we shall speak about "fern-equivalence" and about "fern-equivalent directions".

2. Extremal hypersurfaces and fern-equivalent directions

Let a unit vector $e^\lambda(P)$ represent a given direction at a point P in an n -dimensional riemannian space. It can be either a time-like or a space-like (but not a light-like) vector. In order to define unambiguously which of the directions at another point Q is equivalent ("parallel") to that given by $e^\lambda(P)$ let us make the following construction. We introduce an $(n-1)$ -dimensional minimal (extremal) hypersurface with the following properties: (i) the point P is lying on this hypersurface, (ii) this hypersurface is orthogonal to $e^\lambda(P)$. If the point Q is lying on the same surface then the direction orthogonal to it at the point Q is to be regarded as equivalent, i.e. parallel in the generalized sense of this word, to that represented by $e^\lambda(P)$. Introducing the unit vector $e^\lambda(Q)$ orthogonal to the above mentioned hypersurface and directed so that $e^\lambda(Q)$ goes continuously into $e^\lambda(P)$ for $P \rightarrow Q$ (i.e. pointing to the same side of the hypersurface), the vectors $e^\lambda(P)$ and $e^\lambda(Q)$ can be called fern-equivalent.

In the limit of flat space the minimal hypersurface goes over into a hyperplane and the directions $e^\lambda(Q)$ and $e^\lambda(P)$ become parallel so that, indeed, it means a natural generalization of the notion of parallelism.

If the point Q is not lying on the above mentioned hypersurface then we make the following construction. We introduce a one-parametric family of extremal hypersurfaces

$$\varphi(x^\mu) = p, \quad (1)$$

where φ is a scalar function and p is a parameter, so that

$$\varphi(x^\mu) = p_0 \quad (1')$$

denotes the particular hypersurface introduced formerly. The function φ is restricted by the condition

$$0 < |h^\nu h_\nu| \leq M \quad (2)$$

where

$$h_\nu = \partial_\nu \varphi \quad (3)$$

for every point in the whole space. The family of extremal hypersurfaces satisfying (2)

and (3) will be called "uniform"¹. Now, the versor of the vector h^p

$$e^\mu = |h^p h_p|^{-1/2} h^\mu \quad (4)$$

taken at an arbitrary point Q represents a fern-equivalent direction to that represented by the original $e^\lambda(P)$. In this way we defined a field of fern-equivalent unit vectors e^λ .

In the limit of flat space the one-parametric family of extremal hypersurfaces goes over into a one-parametric family of hyperplanes. In particular, a one-parametric family satisfying (2) goes over into a family of parallel hyperplanes. Hence, the vector field e^λ goes over into a constant vector field. Thus, our definition of fern-equivalence is a natural generalization of the concept of parallelism for the case of riemannian spaces. This generalization is as natural as e.g. the generalization of straight lines to geodesic lines. Both generalizations are of a similar type since both take advantage of the extremal properties inherent in the riemannian geometry. Geodesic lines are one-dimensional extremal manifolds whereas we have exploited now the $(n-1)$ -dimensional extremal manifolds.

As a by-product we get another generalization of the concept of straight lines, quite different from geodesic lines: the orthogonal trajectories to a one-parametric family of $(n-1)$ -dimensional, extremal, uniform hypersurfaces.

According to a theorem of Bianchi (1903) and Bompiani (1921) a necessary and sufficient condition that the family of hypersurfaces (1) be extremal is that their orthogonal trajectories determine a correspondence between them which preserves volume. From this theorem it follows that

$$e^\lambda_{;\lambda} = 0. \quad (5)$$

Thus, our family of extremal hypersurfaces is characterized by a curl-free vector field (3) whose versors form a source-free field. In the next sections we shall exploit mainly the analytical properties (3), (4), and (5).

3. Fern-equivalent tetrads and quasi-cartesian coordinates

Let us introduce four independent uniform families of extremal hypersurfaces

$$\varphi^a = p^a, \quad a = (1), \dots (4), \quad (6)$$

in the four-dimensional riemannian manifold to be interpreted physically as space-time, and assume three of the families to be time-like (for $a=(1), (2),$ and (3)), and the fourth to be space-like (for $a=(4)$). Introducing the vectors h^λ_a and their versors e^λ_a according to (2), (3), and (4), we get a source-free tetrad field

$$e^\lambda_{;\lambda} = 0 \quad (5')$$

satisfying the conditions of normalization but not of orthogonality

$$e^{\lambda a} e^\lambda_b = \gamma^{ab} \quad (7)$$

¹ Uniform families of minimal hypersurfaces surely exist in spaces which become flat for points tending to infinity in space-like directions.

where

$$\gamma^{(11)} = \gamma^{(22)} = \gamma^{(33)} = -\gamma^{(44)} = 1 \quad (7')$$

but

$$\gamma^{ab} = \gamma^{ba} \neq 0 \text{ for } a \neq b. \quad (7'')$$

Such a field of fern-equivalent tetrads will be useful for physical interpretation.

Two observers situated at P and Q whose world lines are just tangential to two orthogonal trajectories of a uniform family of extremal hypersurfaces $\varphi^{(4)} = p$, i.e. whose directions are (momentarily) $e^{\lambda(4)}(P)$ and $e^{\lambda(4)}(Q)$, may be regarded as being at rest one relatively to the other. Thus, it is possible to introduce the concept of a quasi-inertial frame of reference by forcing the bodies of reference to move along the orthogonal trajectories of a uniform family of space-like extremal hypersurfaces. A transition from one quasi-inertial frame of reference to another is done by going over to another family $\varphi'_{(4)} = p$ of the same type.

It is also possible to introduce a quasi-cartesian system of reference by defining the invariant coordinates

$$r^a = \int_{P_0}^P h^a_{\lambda} \frac{dx^{\lambda}}{ds} ds. \quad (8)$$

Owing to (3) the above integrals are independent of the path of integration and can be written also as

$$r^a = \int_{P_0}^P d\varphi^a = \varphi^a(P) - \varphi^a(P_0). \quad (9)$$

If the space-time is of such a type that for $P \rightarrow \infty$ in space-like directions the manifold becomes flat and if we assume additionally

$$h^{\lambda a} h^b_{\lambda} \rightarrow \eta_{ab} \quad (10)$$

for $P \rightarrow \infty$ in space-like directions, then the coordinates r^a become a natural generalization of cartesian coordinates. A transition between two quasi-cartesian systems of reference $r_a \rightarrow r'_a$ is achieved by making a Lorentz transformation of the basic vectors at space-like infinity.

Let us introduce the reciprocal tetrad field $e_{\lambda a}$ by

$$e^{\lambda}_a e^{\lambda}_b = \delta^a_b \quad \text{whence} \quad e^a_{\lambda} e^{\mu}_a = \delta^{\mu}_{\lambda}. \quad (11)$$

It satisfies the relations

$$e^a_{\lambda} e^{b\lambda} = \gamma^{ab} \quad \text{where} \quad \gamma^{ac} \gamma_{cb} = \delta^a_b. \quad (12)$$

Differentiating the second formula (11) with respect to x^{μ} and taking into account (5) we get the useful formula

$$e^{\mu}_a \partial_{\mu} e^a_{\lambda} = \Gamma^{\mu}_{\mu\lambda} \quad (13)$$

4. Local conservation laws in general relativity

In spite of numerous efforts in the past forty five years the problem of local conservation laws for energy-momentum and angular momentum in general relativity has not been solved yet. In view of this situation several physicists represent the opinion that local conservation laws cannot exist since the riemannian space-time is neither homogeneous nor isotropic. We are not convinced by this argument. Conservation laws are violated if the lagrangian depends explicitly on the arguments x^μ , which is not the case in general relativity. The lagrangian of general relativity depends only implicetly upon the arguments x^μ through the intermediary of the field quantities $g_{\mu\nu}$. Conservation laws in special relativity are derivable either directly, by guessing the form of the conserved quantities, or with the help of the well known procedure of infinitesimal rigid displacements. Such rigid displacements are believed to be impossible in the riemannian space. In fact, it is impossible to displace rigidly the riemannian space into itself, i.e. without going beyond it, but surely it is possible to displace it rigidly within the ten-dimensional embedding space. If all material bodies (fields) including the gravitational field itself are rigidly displaced in the embedding space then the observers can use new coordinates and new tetrads displaced so that no change will be noticed except for an immaterial change of notation. Therefore the existence of local conservation laws is to be expected also within the framework of general relativity.

In order to show the possibility of securing localization and conservation of energy, momentum, and of angular momentum we shall not take advantage of the possibility of performing rigid displacements in the embedding space, but we shall use the tetrad technique and the concept of fernequivalence.

From the purely technical point of view the trouble with the conservation laws in general relativity is that the covariant continuity equations

$$G^{\mu\nu}_{;\nu} = 0, \quad (14)$$

where $\frac{1}{\kappa} G^{\mu\nu}$ is the symmetrical energy-momentum-stress tensor

$$\frac{1}{\kappa} G^{\mu\nu} \equiv \frac{1}{\kappa} \left(R^{\mu\nu} - \frac{1}{2} g^{\mu\nu} R \right) = T^{\mu\nu} \quad (15)$$

are not suitable for an application of the Gauss-Ostrogradzki theorem. However, as is well known, there is no difficulty whatsoever with the conservation and localization of the electric charge in general relativity in spite of the fact that in this case we have also to do with a covariant form of the continuity equation. The technical reason for the lack of any difficulty with the charge and an apparently insurmountable difficulty with the energy-momentum is due to the fact that covariant derivatives mean something else for each case of tensors of different ranks. The case of tensors of the first rank T^μ is, so to say, natural for deriving conservation laws from covariant continuity equations.

$$T^\mu_{;\mu} = 0. \quad (16)$$

Indeed by integrating (16) over an arbitrary four-dimensional volume Ω , we get an expression to which the Gauss theorem is directly applicable

$$0 = \int_{\Omega} (\partial_{\mu} T^{\mu} + \Gamma_{\mu\nu}^{\mu} T^{\nu}) \sqrt{-g} dx = \int_{\Omega} \partial_{\mu} (T^{\mu} \sqrt{-g}) dx = \sum_{(\mu\nu\varrho\sigma)} \oint_{\Sigma} T^{\mu} \sqrt{-g} dS^{\nu\varrho\sigma} \quad (17)$$

where use was made of the well known formula

$$\partial_{\mu} \sqrt{-g} = \Gamma_{\mu\nu}^{\nu}. \quad (18)$$

Introducing the element dS_{μ} dual to $dS^{\nu\varrho\sigma}$

$$dS_{\mu} = \sqrt{-g} dS^{\nu\varrho\sigma}, \quad (19)$$

splitting the closed hypersurface into two space-like hypersurfaces Σ_1 and Σ_2 , changing the direction of the normal on Σ_2 , we get

$$\int_{\Sigma_1} T^{\mu} dS_{\mu} = \int_{\Sigma_2} T^{\mu} dS_{\mu}, \quad (20)$$

whence the quantity

$$T = \int_{\Sigma} T^{\mu} dS_{\mu} = \int_{\Sigma} T^{\mu} dS \quad (21)$$

is independent of the choice of the space-like hypersurface, i.e. is conserved. The normal component T^n is interpretable as the density of T at the points of Σ .

In the above derivation the form of the covariant derivative of the vector was explicitly taken advantage of. In the case of tensors of higher ranks $T^{\mu\nu\dots}$, where the covariant derivatives involve further terms with Christoffel symbols, the analogous derivation obviously breaks down and it is impossible to infer the conservation laws.

The above discussion not only shows where technical difficulties arise from but, at the same time, suggest the way out of the difficulties: The tensor of energy-momentum is to be replaced by a suitable set of vectors. This end can be achieved by using the tetrad technique. By means of projections upon the legs of the four-leg (tetrad) $h^{a\mu}$ we can replace the energy-momentum-stress tensor $W^{\mu\nu}$ of the complete system including substantialistic matter as well as gravitation by a set of four fourvectors

$$W^{\mu a} = h^{a\nu} W_{\nu}^{\mu}. \quad (22)$$

These vectors may be called the energy-momentum "currents".

If we succeed in satisfying continuity equations of the following form

$$W_{;\mu}^{\mu a} = 0 \quad (23)$$

then, repeating exactly the derivation (16)–(21), we shall find strictly conserved and localizable quantities

$$W^a = \int_{\Sigma} W^{a\mu} dS_{\mu} \quad (24)$$

to be interpreted as the total energy-momentum components with respect to the tetrad field $h^{a\lambda}$. The normal components W_a^n will be interpretable as the corresponding densities.

Thus, in order to guarantee conservation and strict localization of energy-momentum in general relativity, we have to construct the "currents" satisfying the continuity equations (23). It is obviously possible to find a symmetrical tensor $W_{\mu\nu}$ satisfying (23), i.e. to guarantee local conservation laws for energy-momentum. However, as there are ten unknown functions $W_{\mu\nu}$ and only four equations (23), the problem is still underdetermined. In order to determine $W_{\mu\nu}$ from (23) some more information about the structure of $W_{\mu\nu}$ is needed.

$W^{\mu\nu}$ can be defined as

$$W_{\mu\nu} = h_a^\mu \Theta^{ab} h_b^\nu \quad (25)$$

where Θ_b^a is the generator of infinitesimal translations of quasi-inertial coordinates r^a . The generator Θ^{ab} is identical with the well known affine tensor of Einstein if (and only if) the latter is expressed in quasi-inertial coordinates. But Θ^{ab} has a covariant meaning: it is a set of scalars with respect to general coordinate transformations and transforms like a tensor with respect to transformations replacing one system of families of extremal hypersurfaces by another system of extremal hypersurfaces.

The tensor $W^{\mu\nu}$ can be symmetrized by the well known procedure of Belinfante which secures local conservation laws of the quantities

$$M^{ab\mu} = r^a W^{b\mu} - r^b W^{a\mu},$$

representing angular momentum.

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THE GENERALIZATION OF DIRAC'S EQUATION II

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The quantized Lagrangian formalism, which leads to the generalized Dirac equation introduced in I, is investigated. The theory is invariant with respect to the 12-parameter $C \times C'$ group. The Lagrangian is described by means of the two real isovectors: the mass-isovector $\kappa_{;\mu}$ (introduced in I) and a second isovector $\epsilon'_{;\mu}$ not occurring in the equation. The isovector $\epsilon'_{;\mu}$ is necessary for quantization invariant under $C \times C'$. It is shown that the Jauch field may be obtained and generalized after a special choice of $\epsilon'_{;\mu}$.

Introduction

In the present paper we continue some considerations published recently (Lukierski 1960¹) was to introduce the generalized Dirac equation, invariant under to the 12-parameter group $C \times C'$. We have stated on a generalized Dirac equation described with help of an isovector $\kappa_{;\mu}$ standing for the scalar mass in the usual Dirac equation. It is also shown that if the mass-isovector is chosen as follows (see (I.1.15)):

$$\kappa_{;\mu} = (0, 0, -m, 0) \quad (0.1)$$

we obtain the conventional Dirac equation.

In the following considerations we go over to the quantized theory. The most general Lagrangian, invariant under the $C \times C'$ group, bilinear in the field operators $\Psi_{\alpha;\beta}$, $\Psi_{\alpha;\beta}^+$, and linear in the derivatives (Sect. 1,2) leads to the equation investigated in I (Sect 3). The formulation of the Lagrangian formalism with help of the 8-spinor notation yields a possibility of quantization (Sect. 4,5).

The Lagrangian for our general equation is not determined uniquely. We obtain three new degrees of freedom, described by means of the coordinates of a second isovector $\epsilon'_{;\mu}$, which satisfy the following relation (Sect. 7):

$$\kappa_{;\mu} \epsilon'_{;\mu} = 0 \quad (0.2)$$

¹ Quoted hereafter as I.

The introduction of the second isovector $\epsilon'_{i\mu}$ permits to interpret the Jauch field (Jauch 1954); this field is obtained as a special case of our generalized field (Sect. 6). Schwinger's choice of the Lagrangian (Schwinger 1948) implies (besides (0.1)):

$$\epsilon'_{i\mu} = (0, 0, 0, 1) \quad (0.3)$$

and for the Jauch field we get

$$\epsilon'_{i\mu} = (\beta, 0, 0, \alpha) \quad \alpha^2 - \beta^2 = 1 \quad (0.4)$$

We see also that the Jauch field for which

$$\begin{aligned} \{\bar{\psi}(x), \psi(x')\} &= -iS_{\alpha\beta}(x-x'), \\ \{\hat{\psi}(x), \psi(x')\} &= -i\rho S_{\alpha\beta}(x-x'), \end{aligned} \quad (0.5)$$

where $\hat{\psi} \equiv \psi\gamma_4$ and

$$0 \leq \varrho \leq 1 \quad \varrho = \varrho^* \quad (0.5a)$$

can be generalized to the 2-parameter Jauch field, for which instead of (0.5a)

$$0 \leq |\varrho| < 1 \quad \varrho \neq \varrho^* \quad (0.5b)$$

Let us finally enumerate some fields introduced in the last years as generalized Dirac fields. These fields are described with help of our generalized equation:

A. The *Ozaki field* (Ozaki 1960), introduced by the following equation

$$\{\gamma_\mu \partial_\mu - e^{\beta\gamma_5} m\} \psi = 0 \quad (0.6)$$

where $\beta = \beta^*$, can be obtained by putting

$$\epsilon_{i\mu} = (0, 0, \cosh \beta, \sinh \beta) \quad (0.7)$$

Equation (0.6) was also introduced in another form by Woythousen (1958).

B. The *Lurie field* (Lurie 1959), obtained from the conventional Dirac field by using the following 4-parameter subgroup of C'

$$\psi' = e^{\beta\gamma_5} (a\psi + b\gamma_5\psi^c) \quad (0.8)$$

where

$$\beta = \beta^* \quad |a|^2 + |b|^2 = 1 \quad (0.8a)$$

and the upper index "c" denotes charge conjugation.

C. The *Jauch field* (Jauch 1954), described by means of (0.1) and (0.4).

D. If, according to a proposal of Rzewuski (1958), we introduce in spinor space the following 1-parameter group

$$a: \quad \Psi'_{\alpha;\beta} = e_{i\alpha} \Psi_{\alpha;\beta} \quad (0.9)$$

we obtain the *Nishijima field* in the conventional 4-spinor Dirac equation,

$$\{\gamma_\mu \partial_\mu - e^{i\alpha\gamma_5} m\} \psi = 0 \quad (\alpha = \alpha^*), \quad (0.10)$$

a field introduced for leptons by Nishijima (1957).

1. Bilinear Forms Constructed from Spinor-Isospinors

It is easily seen that from the simplest true non-hermitian representation $\Psi_{\alpha;\beta}$ of the $C \times C'$ group (see I) one can construct² only the following five bilinear tensor forms in $C \times C'$:

$$T = \Psi_{\alpha;\beta} \Psi^{\alpha;\beta} \quad (1.1)$$

$$T_{\mu\varrho;\gamma} = \Psi_{\alpha;\beta} T_{\mu\varrho;\gamma}^{\alpha} \Psi^{\gamma;\beta} \quad (1.2)$$

$$T_{;\nu\tau} = \Psi_{\alpha;\beta} T_{;\nu\tau}^{\beta} \Psi^{\alpha;\delta} \quad (1.3)$$

$$T_{\mu;\nu} = \Psi_{\alpha;\beta}^+ \sigma_{\mu;\dot{\alpha}}^{\gamma} \sigma_{\nu;\dot{\beta}}^{\delta} \Psi_{\gamma;\delta} \quad (1.4)$$

$$T_{\mu\varrho;\nu\tau} = \Psi_{\alpha;\beta} T_{\mu\varrho;\gamma}^{\alpha} T_{;\nu\tau}^{\beta} \Psi^{\gamma;\delta} \quad (1.5)$$

where

$$T_{\mu\varrho;\gamma}^{\alpha} = \frac{1}{2} (\sigma_{\mu;\dot{\alpha}}^{\beta} \sigma_{\varrho;\dot{\beta}\gamma} - \sigma_{\varrho;\dot{\alpha}}^{\beta} \sigma_{\mu;\dot{\beta}\gamma}) \quad (1.6)$$

$$T_{;\nu\tau}^{\beta} = \frac{1}{2} (\sigma_{;\nu}^{\dot{\gamma}\beta} \sigma_{;\tau\dot{\gamma}\delta} - \sigma_{;\tau}^{\dot{\gamma}\beta} \sigma_{;\nu\dot{\gamma}\delta}) \quad (1.6)$$

$$\Psi_{\alpha;\beta} \equiv \sigma_{\alpha\gamma;\dot{\sigma}} \sigma_{\beta\delta}^{\gamma} \Psi^{\gamma;\delta} \quad (1.7)$$

$\sigma = \sigma'$ — metric tensor in spinor space (Corson 1954), $\sigma_{\mu;\dot{\alpha}}, \sigma_{\nu;\dot{\beta}}$ — well-known 2×2 Pauli matrices.

It may be proved that in classical theory

$$T_{\mu\varrho} = T_{;\nu\tau} = T_{\mu\varrho;\nu\tau} \equiv 0 \quad (1.8)$$

and

$$\begin{aligned} T_{\mu;\alpha} T^{\mu;\beta} &= T T^* \delta_{\alpha\beta} \\ T_{\gamma;\nu} T^{\epsilon;\nu} &= T T^* \delta_{\gamma\epsilon} \end{aligned} \quad (1.9)$$

From (1.9) we obtain Takabayashi's Lorentz frame of $\frac{1}{2}$ -spin particle (Takabayashi 1958a, b).

Let us consider the non-commuting field operators $\Psi_{\alpha;\beta}, \Psi_{\alpha;\beta}^+$. Because

$$T_{\mu\varrho;\gamma}^{\alpha} \equiv \frac{1}{2} \epsilon_{\mu\varrho\tau\kappa} T_{\tau\kappa;\gamma}^{\alpha} \quad (1.10)$$

and analogously for $T_{;\nu\tau}^{\alpha}$, the antisymmetrical tensors $T_{\mu\varrho;\gamma}, T_{;\nu\tau}$ and $T_{\mu\varrho;\nu\tau}$ are fully determined by their space and isospace components:

$$T_{4i} \equiv -\frac{1}{2} \epsilon_{ijk} T_{jk}; \quad (1.11a)$$

$$T_{;4i} \equiv -\frac{1}{2} \epsilon_{ijk} T_{;jk} \quad (1.11b)$$

$$T_{4i;4r} \equiv \frac{1}{4} \epsilon_{ijk} \epsilon_{rst} T_{jk;st} \quad (1.11c)$$

² We indicate the components in C with an index before the semicolon, and the components in C' — with an index behind the semicolon. Because all the spin-tensors investigated below belong to usual or iso-space, it is sufficient to indicate with semicolon the tensor indices only.

We see also that the transposition operation (classically equal to the identity transformation) leads to the following equalities:

$$\begin{aligned} T^T &\equiv T & T_{ij;kl}^T &\equiv T_{ij;kl} \\ T_{ij}^T &\equiv -T_{ij} & T_{ij} &\equiv -T_{ij} \\ T_{\mu;\nu}^T &= \Psi_{\alpha;\beta} \sigma_{\mu;\alpha}^T \sigma_{\nu;\beta}^T \Psi_{\gamma;\delta} \end{aligned} \quad (1.12)$$

where only $T_{\mu;\nu}$ and $T_{\mu;\nu}^T$ are independent.

Taking into account the hermiticity of the tensors (1.1-5), it is easily seen that only $T_{\mu;\nu}$ is hermitian. Thus from each form (1.1-5) we obtain two different hermitian tensors, which are scalar or pseudoscalar with respect to the transposition operation (1.12):

$$T^{(+)} = \frac{1}{2} (T + T^+) \quad T^{(-)} = \frac{i}{2} (T - T^+) \quad (1.13a)$$

$$T_{ijl}^{(+)} = \frac{i}{2} (T_{ijl} - T_{ijl}^+) \quad T_{ijl}^{(-)} = \frac{1}{2} (T_{ijl} + T_{ijl}^+) \quad (1.13b)$$

$$T_{ikj}^{(+)} = \frac{i}{2} (T_{ikj} - T_{ikj}^+) \quad T_{ikj}^{(-)} = \frac{1}{2} (T_{ikj} + T_{ikj}^+) \quad (1.13c)$$

$$T_{\mu;\nu}^{(\pm)} = \frac{1}{2} (T_{\mu;\nu} \pm T_{\mu;\nu}^T) \quad (1.13d)$$

$$T_{ikj;jl}^{(+)} = \frac{1}{2} (T_{ikj;jl} + T_{ikj;jl}^+)$$

$$T_{ikj;jl}^{(-)} = \frac{i}{2} (T_{ikj;jl} - T_{ikj;jl}^+). \quad (1.13e)$$

Let us introduce the following transformation

$$\hat{K} \Psi_{\alpha;\beta} = (\Psi_{\alpha;\beta})^+, \quad (1.14)$$

which commute with the unitary subgroup $U \times U'$. If we put

$$\hat{K} = I_4 \cdot I_4', \quad (1.15)$$

we see that $T_{\mu;\nu}^{(+)}$ describe tensors, and $T_{\mu;\nu}^{(-)}$ — pseudotensors with respect to the inversions of time and isotime, defined with help of formula (1.14).

2. The General Lagrangian

The most general bilinear Lagrangian leading to the first order equation for $\Psi_{\alpha;\beta}$, which is invariant with respect to the group $C \times C'$, is the following one:

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 \quad (2.1)$$

where

$$\mathcal{L}_1 = \frac{i}{2} (\alpha \Psi_{\alpha;\beta}^+ \delta^{\alpha\gamma;\beta\delta} \Psi_{\gamma\delta} + \beta \Psi_{\alpha;\beta} \hat{c}^{\alpha\gamma;\beta\delta} \Psi_{\gamma\delta}^+) \quad (2.2)$$

$$\mathcal{L}_2 = \frac{a}{2} \Psi_{\alpha;\beta} \Psi^{\alpha;\beta} + \text{H.C.} \quad (2.3)$$

$$\mathcal{L}_3 = \frac{b}{2} \Psi_{\alpha;\beta} E^{\beta;\delta} \Psi_{\alpha;\delta} + \text{H.C.} \quad (2.4)$$

where α, β are real, and a, b complex.

If we introduce

$$\epsilon^{;\dot{\beta}\delta} = \sigma_{;\mu}^{\dot{\beta}\delta} \epsilon_{;\mu} \quad (2.5)$$

after putting

$$\tilde{\epsilon}^{;\beta\dot{\delta}} = (\epsilon^{;\dot{\beta}\delta})^* \quad (2.6)$$

we have from the hermiticity condition for \mathcal{L}_1 ,

$$\epsilon_{;l} = \epsilon_{;l}^* \quad \epsilon_{;4} = -\epsilon_{;4}^* \quad (2.7)$$

If we suppose that

$$E^{;\beta\delta} = E^{;\delta\beta} \quad (2.8)$$

the tensor $E_{;\mu\nu}$, obtained from $E^{;\beta\delta}$ with help of the formula

$$E^{;\beta}_{\delta} = \frac{1}{2} T_{;\mu\nu}^{\beta} E_{;\mu\nu} \quad (2.9)$$

may be assumed to be antisymmetrical and real³:

$$E_{;lk} = E_{;lk}^* \quad E_{;4l} = -E_{;4l}^* \quad (2.10)'$$

Further limitations on (2.1) follow from the consistency of the two equations

$$\frac{\delta \mathcal{L}}{\delta \Psi_{\alpha;\beta}} \equiv i\beta \epsilon^{;\alpha\gamma;\delta} \epsilon^{;\beta\delta} \Psi_{\gamma;\delta}^+ + a \Psi^{\alpha;\beta} + b E^{;\beta}_{\delta} \Psi^{\alpha;\delta} = 0 \quad (2.11)$$

$$\frac{\delta \mathcal{L}}{\delta \Psi_{\alpha;\beta}^+} \equiv i\alpha \epsilon^{;\alpha\gamma;\delta} \epsilon^{;\beta\delta} \Psi_{\gamma;\delta} + a^* (\Psi^{\alpha;\beta})^+ - b^* (E^{;\beta}_{\delta})^* (\Psi^{\alpha;\delta})^+ = 0 \quad (2.12)$$

where the variations are taken from the left. Writing out the complex conjugate equation of (2.12):

$$-i\alpha \epsilon^{;\alpha\gamma;\delta} \epsilon^{;\beta\delta} \Psi_{\gamma;\delta}^+ + a \Psi^{\alpha;\beta} - b E^{;\beta}_{\delta} \Psi^{\alpha;\delta} = 0 \quad (2.13)$$

we obtain following the restrictions on the parameters in (2.1):

$$\begin{array}{lll} \text{A) } \alpha = -\beta & a \neq 0 & b = 0 \\ \text{B) } \alpha = \beta & a = 0 & b \neq 0 \end{array} \quad (2.14)$$

³ It is also possible to assume the self-duality condition, which implies three independent complex components satisfying (1.11b).

which lead to the following two Lagrangians

$$\mathcal{L}_A = \frac{i}{2} (\Psi_{\alpha;\beta}^+ \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon^{;\beta\delta} \Psi_{\gamma;\delta} - \Psi_{\alpha;\beta} \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon^{;\beta\delta} \Psi_{\gamma;\delta}^+) + \left(\frac{a}{2} \Psi_{\alpha;\beta} \Psi^{\alpha;\beta} + H.C. \right) \quad (2.15)$$

$$\mathcal{L}_B = \frac{i}{2} (\Psi_{\alpha;\beta}^+ \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon'^{;\beta\delta} \Psi_{\gamma;\delta} - \Psi_{\alpha;\beta} \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon'^{;\beta\delta} \Psi_{\gamma;\delta}^+) + \left(\frac{b}{2} \Psi_{\alpha;\beta} E^{;\beta}{}_{\delta} \Psi^{\alpha;\delta} + H.C. \right) \quad (2.16)$$

Using (1.13-15), it is easily seen that if

$$a = -a^* \quad b = -b^* \quad (2.17a)$$

we have

$$\begin{aligned} \hat{K} \mathcal{L}_A \hat{K}^{-1} &= -\mathcal{L}_A \\ \hat{K} \mathcal{L}_B \hat{K}^{-1} &= \mathcal{L}_B \end{aligned} \quad (2.17b)$$

thus the Lagrangians \mathcal{L}_A , \mathcal{L}_B have the determined parities.

The equations obtained from (2.15) and (2.16) are

$$\hat{R}_1^{\alpha\gamma;\beta\delta} \Psi_{\gamma;\delta} \equiv i \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon^{;\beta\delta} \Psi_{\gamma;\delta}^+ - a \Psi^{\alpha;\beta} = 0 \quad (2.18)$$

$$\hat{R}_2^{\alpha\gamma;\beta\delta} \Psi_{\gamma;\delta} \equiv i \hat{\mathcal{C}}^{\alpha\gamma}; \epsilon'^{;\beta\delta} \Psi_{\gamma;\delta}^+ + b E^{;\beta}{}_{\delta} \Psi^{\alpha;\delta} = 0 \quad (2.19)$$

If we put

$$\epsilon'^{;\beta\delta} = -\frac{b}{a} E^{;\beta}{}_{\gamma} \epsilon^{;\gamma\delta}, \quad (2.20)$$

we have

$$\hat{R}_2^{\alpha\gamma;\beta\delta} = E^{;\beta}{}_{\epsilon} \hat{R}_1^{\alpha\gamma;\epsilon\delta} \quad (2.21)$$

and if

$$|E^{;\beta}{}_{\gamma}| = E_{;\mu\nu} E^{;\mu\nu} \neq 0 \quad (2.22)$$

the equation (2.19) can be obtained from (2.18).

Introducing (0.9), where

$$[\mathbf{c}, \mathbf{a}] = [\mathbf{c}', \mathbf{a}] = 0 \quad (2.23)$$

we see that under this transformation in (2.1)

$$\begin{aligned} a &\rightarrow a' = e^{-i2\alpha} a \\ b &\rightarrow b' = e^{-i2\alpha} b, \end{aligned} \quad (2.24)$$

and taking into account the group \mathbf{a} , the conditions (2.17a) might be always satisfied. Therefore, the equations (2.18-19) are invariant under (1.13).

3. The Correspondence with the Klein-Gordon Equation

Let us assume that

$$(\square - m^2)\Psi_{\alpha;\beta} = 0 \quad (3.1)$$

From (2.18) we obtain

$$-i\partial_{\alpha;\gamma}\epsilon_{\beta\delta}\Psi^{\gamma\delta} - a^*\Psi_{\alpha;\beta}^+ = 0 \quad (3.2)$$

and, using

$$\begin{aligned} \partial_{\epsilon\alpha}\epsilon^{\alpha\gamma} &= -\square\delta_{\epsilon}^{\gamma} \\ \epsilon_{\beta\tau}\epsilon^{\beta\delta} &= -\epsilon_{\beta\tau}^2\delta^{\beta\delta} \end{aligned} \quad (3.3)$$

we have from (2.18) and (3.2)

$$(\epsilon_{\beta\mu}^2 \square - |a|^2)\Psi_{\alpha;\beta}^+ = 0 \quad (3.4)$$

The equations (3.1) and (3.4) are equivalent, if

$$m^2 = \frac{|a|^2}{\epsilon_{\beta\mu}^2} \quad (3.5)$$

From the relation (3.5), we see that

$$\epsilon_{\beta\mu}^2 = \epsilon_{\beta l}^2 - \epsilon_{\beta o}^2 > 0 \quad (3.6)$$

and

$$\kappa_{\beta\mu} = \frac{m}{\sqrt{\epsilon_{\beta\mu}^2}}\epsilon_{\beta\mu} = \frac{|a|}{\epsilon_{\beta\mu}^2}\epsilon_{\beta\mu} \quad (3.7)$$

is the mass-isovector, introduced in I, for which

$$\kappa_{\beta\mu}^2 = m^2 \quad (3.8)$$

It is easily seen that after multiplication of (2.18) by $i\epsilon_{\beta\tau}$, we obtain

$$\partial^{\alpha\gamma}\Psi_{\gamma\tau}^+ - A\kappa_{\beta\tau}\Psi^{\alpha\beta} = 0 \quad (3.9)$$

where

$$A = -i\frac{a}{|a|} \quad (3.9a)$$

and

$$|A|^2 = 1 \quad (3.9b)$$

accordingly to the results of I.

Let us investigate the correspondence of (2.19) with the Klein-Gordon equation. If

$$E_{\beta}^{\delta} = (E_{\beta\delta})^* \quad (3.10)$$

the complex conjugate equation to (2.19) is

$$-i\partial_{\alpha\gamma}\epsilon'_{\beta\delta}\Psi^{\gamma\delta} - b^*E_{\beta\delta}^{\cdot\dot{\beta}}\Psi_{\alpha\delta}^+ = 0 \quad (3.11)$$

Now we multiply (2.19) by $\partial_{\alpha\gamma}\epsilon'_{\beta\delta}$ and (3.11) by $-ibE_{\beta\delta}^{\cdot\dot{\beta}}$ and obtain by addition

$$i\epsilon_{\beta\mu}^{\prime 2}\square\Psi_{\epsilon\tau}^+ + b\partial_{\alpha\gamma}(\epsilon'_{\beta\tau}E_{\gamma\delta}^{\beta\delta} - E_{\beta\tau}^{\cdot\dot{\beta}}\epsilon'_{\gamma\delta})\Psi^{\alpha\delta} - ib^2E_{\beta\tau}^{\cdot\dot{\beta}}E_{\gamma\delta}^{\cdot\dot{\delta}}\Psi_{\epsilon\delta}^+ = 0 \quad (3.12)$$

From the relation (2.9) we have

$$E_{\beta\tau}^{\cdot\dot{\beta}}E_{\gamma\delta}^{\cdot\dot{\delta}} = -(E_{\beta\mu\nu}E_{\gamma\mu\nu} + iE_{\beta\mu\nu}\check{E}_{\gamma\mu\nu})\delta_{\gamma\tau}^{\cdot\dot{\delta}} \quad (3.13)$$

where

$$\check{E}_{\beta\mu\nu} = \frac{1}{2i}\epsilon_{\mu\nu\lambda\kappa}E_{\beta\lambda\kappa} \quad (3.14)$$

By virtue of (3.12-14) we see that if

$$\epsilon'_{\beta\tau}E_{\gamma\delta}^{\beta\delta} = E_{\beta\tau}^{\cdot\dot{\beta}}\epsilon'_{\gamma\delta} \quad (3.15)$$

and

$$E_{\beta\mu\nu}\check{E}_{\gamma\mu\nu} = 0 \quad (3.16)$$

equation (3.12) is equivalent to (3.1). In this case

$$m^2 = \frac{|b|^2 E_{\beta\mu\nu}E_{\gamma\mu\nu}}{\epsilon_{\beta\mu}^{\prime 2}} \quad (3.17)$$

The supplementary condition (3.15) may be described by help of the isotensor components $\epsilon'_{\beta\gamma}$, $E_{\beta\mu\lambda}$. Because (Corson 1954)

$$\sigma_{\beta\mu\alpha}T_{\gamma\kappa\lambda}^{\beta\delta} = (\delta_{\mu\gamma}^{\kappa\lambda} + \epsilon_{\kappa\lambda\mu\gamma})\sigma_{\gamma\alpha\delta} \quad (3.18a)$$

$$T_{\beta\kappa\lambda}^{\cdot\dot{\beta}}\sigma_{\gamma\mu\delta}^{\beta\delta} = (\delta_{\mu\gamma}^{\kappa\lambda} - \epsilon_{\kappa\lambda\mu\gamma})\sigma_{\gamma\nu\delta} \quad (3.18b)$$

where

$$\delta_{\mu\gamma}^{\kappa\lambda} = \delta_{\mu\kappa}\delta_{\gamma\lambda} - \delta_{\mu\lambda}\delta_{\gamma\kappa} \quad (3.19)$$

we have

$$\epsilon'_{\beta\tau}E_{\gamma\delta}^{\beta\delta} = \epsilon'_{\beta\mu}(E_{\gamma\mu\nu} + i\check{E}_{\gamma\mu\nu})\sigma_{\nu\tau\delta} \quad (3.20a)$$

$$E_{\beta\tau}^{\cdot\dot{\beta}}\epsilon'_{\gamma\delta} = \epsilon'_{\beta\mu}(E_{\gamma\mu\nu} - i\check{E}_{\gamma\mu\nu})\sigma_{\nu\tau\delta} \quad (3.20b)$$

and (3.15) implies that

$$\epsilon'_{\beta\mu}\check{E}_{\gamma\mu\nu} = 0 \quad (3.21)$$

It is shown in Appendix I that the limitation (3.16) follows from (3.21). Therefore the supplementary condition (3.21) describes all limitations on the isotensor components in \mathcal{L}_B .

Let us multiply (2.19) by $i\epsilon'_{;\tau\beta}$. We obtain thus equation (3.9), where

$$\kappa_{;\tau\delta} = -|b|\epsilon'_{;\tau\beta}E^{\beta}_{\delta} \quad (3.22a)$$

and

$$A = -i \frac{b}{|b|} \quad (3.22b)$$

Considering (3.20a) and (3.22a), we see that our supplementary condition (3.21) is equivalent to the reality condition of the mass-isovector $\kappa_{;\mu}$. It may be also noted that in the equation (2.21) the isovector $\epsilon_{;\mu}$ from $\hat{\mathbf{R}}_1$ can be chosen real only if relation (3.21) is satisfied. Indeed, from (2.20) we have

$$\epsilon_{;\gamma\delta} = -\frac{a}{bE^{\lambda}_{\beta}E^{\beta}_{\lambda}}E^{\gamma\gamma}_{\beta}\epsilon'_{;\beta\delta} \quad (3.23)$$

or, by virtue of (3.10) and (3.20b)

$$\epsilon_{;\nu} = \frac{a}{bE^{\lambda}_{\beta}E^{\beta}_{\lambda}}\epsilon'_{;\mu}(E_{;\mu\nu} + i\check{E}_{;\mu\nu}) \quad (3.24)$$

By assuming (3.21), we obtain

$$\epsilon_{;\nu} = -\frac{a}{b}\epsilon'_{;\mu}\frac{E_{;\mu\nu}}{E_{;0\lambda}E_{;0\lambda}} \quad (3.25)$$

where if

$$\text{Im}\left(\frac{a}{b}\right) = 0 \quad (3.25a)$$

the isovector $\epsilon_{;\mu}$ is also real.

Finally we conclude that \mathcal{L}_A and \mathcal{L}_B with the supplementary condition (3.21) implies the generalized Dirac equation introduced in I.

4. The 8-spinor Notation

Let us introduce the 8-spinor Φ (see I.4.6), which satisfies the following supplementary condition

$$\Phi \equiv i\tau_2\Gamma_5\mathcal{L}\bar{\Phi} = A\bar{\Phi} = \hat{A}\Phi \quad (4.1)$$

where

$$\begin{aligned} \tau_i &= \sigma_i \times I_4 & \Gamma_\mu &= I_2 \times \gamma_\mu \\ \gamma_i &= \varrho_2 \Sigma_i & \gamma_4 &= \varrho_1 \end{aligned} \quad (4.2)$$

and

$$\mathcal{L} = I_2 \times C \quad C = i\varrho_3 \Sigma_2 \quad (4.3)$$

Because

$$\bar{\Phi} = \Phi^\dagger \Gamma_4 = \frac{1}{\sqrt{2}} (\bar{\psi}, -\bar{\psi}^c \gamma_5) \quad (4.4)$$

we obtain from Sect. 1

$$\begin{aligned} T^{(+)} &= \bar{\Phi} \Phi & T^{(-)} &= i \bar{\Phi} \Gamma_5 \Phi \\ T_{;l}^{(+)} &= \frac{1}{2} \epsilon_{ijk} T_{;jk}^{(+)} = \bar{\Phi} \tau_i \Phi \\ T_{;l}^{(-)} &= \frac{1}{2} \epsilon_{ijk} T_{;jk}^{(-)} = i \bar{\Phi} \tau_i \Gamma_5 \Phi \\ T_{\mu;v}^{(+)} &= -i \bar{\Phi} \Gamma_\mu \Gamma_5 \tau_v \Phi \\ T_{\mu;v}^{(-)} &= -i \bar{\Phi} \Gamma_\mu \tau_v \Phi \end{aligned} \quad (4.5)$$

where

$$\tau_v = (\tau_i, -i\Gamma_5) \quad (4.6)$$

The relations (4.5) may be written in an arbitrary γ_μ -representation.

If we substitute in (2.15-16) the tensor forms (4.5), the Lagrangians may be written as follows:

$$\mathcal{L}_A = \bar{\Phi} \Gamma_\mu \partial_\mu \tau_v \epsilon_{;v} \Phi + |a| \bar{\Phi} \exp(i\alpha \Gamma_5) \Phi, \quad (4.7)$$

$$\mathcal{L}_B = \bar{\Phi} \Gamma_5 \Gamma_\mu \partial_\mu \tau_v \epsilon'_{;v} \Phi + |b| \bar{\Phi} \exp(i\beta \Gamma_5) (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau} \Phi, \quad (4.8)$$

where

$$a = |a| e^{i\alpha} \quad b = |b| e^{i\beta} \quad (4.9)$$

and (\vec{E}, \vec{D}) is the following iso-six-vector

$$\begin{aligned} \vec{E} &= (E_{;23}, E_{;31}, E_{;12}) \\ \vec{D} &= (E_{;01}, E_{;02}, E_{;03}) \end{aligned} \quad (4.11)$$

The equations obtained from \mathcal{L}_A and \mathcal{L}_B are as follows:

$$\hat{R}_1 \Phi = (\Gamma_\mu \partial_\mu \tau_v \epsilon_{;v} + |a| e^{i\alpha \Gamma_5}) \Phi = 0 \quad (4.12)$$

$$\hat{R}_2 \Phi = \{\Gamma_5 \Gamma_\mu \partial_\mu \tau_v \epsilon'_{;v} + |b| e^{i\beta \Gamma_5} (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau}\} \Phi = 0 \quad (4.13)$$

From (4.1) we have

$$[\hat{A}, \hat{R}_1] = \{\hat{A}, \hat{R}_2\} = 0 \quad (4.14)$$

The equations (4.12) and (4.13) are identical, if (assuming $\alpha = \beta$)

$$\hat{R}_2 = \frac{b}{a} (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau} \cdot \hat{R}_1 \quad (4.15)$$

The 8-spinor formalism is very useful in investigations of the commutation relations, as the field equations (4.12-13) are linear.

5. The Commutation Relations

The conventional method of Jordan-Pauli-Fierz (Jordan and Pauli 1928, Fierz 1939, Fierz and Pauli 1939) for quantization of a free field is based on the definition of canonical variables. We shall quantize our field without the canonical formalism, using methods, developed by Umezawa and Takahashi (Takahashi and Umezawa 1953, Umezawa 1956). In this method we obtain the commutation relations directly from the field equation, if this equation can be reduced to the Klein-Gordon equation.

Let us have (see Takahashi and Umezawa 1953, eq. (2.1))

$$\mathbf{R}_{\alpha\beta}(\partial_\mu) Q_\beta(x) = 0 \quad (5.1)$$

where (5.1) is obtained from the Lagrangian by taking the variation $\delta\tilde{Q}_\alpha$ from the left.

Thus if

$$\mathbf{R}_{\alpha\beta}(\partial_\mu) \mathbf{D}_{\beta\gamma}(\partial_\mu) = (\square - m^2) \delta_{\alpha\beta} \quad (5.2)$$

we obtain (see Takahashi and Umezawa 1953, eq. (2.3))

$$[\tilde{Q}_\alpha, Q_\beta]_\pm = i\mathbf{D}_{\alpha\beta}(\partial_\mu) \Delta(x - x') \quad (5.3)$$

In our case

$$Q_\alpha \equiv \Phi_A \quad \tilde{Q}_\alpha \equiv \bar{\Phi}_A \quad (5.4)$$

If we assume, in accordance with (3.6),

$$\epsilon_{;v}^2 = 1 \quad (5.5a)$$

and

$$E_{;\mu\nu} E_{;\mu\nu} = \epsilon_1 \quad \epsilon_{;\mu}'^2 = \epsilon_2 \quad (5.5b)$$

where $\epsilon_l^2 = 1$, $l = 1, 2$,

we get from (3.5) and (3.17)

$$m = |a| \quad (5.6a)$$

and

$$m = \epsilon_1 \epsilon_2 |b|, \quad (5.6b)$$

which implies

$$\epsilon_1 \epsilon_2 = 1 \quad (5.7a)$$

or

$$\epsilon_1 = \epsilon_2 = \epsilon \quad (5.7b)$$

From (5.2) and (4.12-13) we have (assuming (5.6))

$$\hat{\mathbf{D}}_1 = \Gamma_\mu \partial_\mu \tau_\nu \epsilon_{;v} - m e^{-i\alpha\Gamma_5} \quad (5.8)$$

$$\hat{\mathbf{D}}_2 = -\epsilon \{ \Gamma_5 \Gamma_\mu \partial_\mu \tau_\nu \epsilon_{;v}' - m e^{-i\beta\Gamma_5} (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau} \} \quad (5.9)$$

It is easy to prove that

$$\hat{R}_1 \hat{D}_1 - \hat{R}_2 \hat{D}_2 = \square - m^2 \quad (5.10)$$

If we define

$$K_{AB}(x-x') = \{\bar{\Phi}_A(x), \Phi_B(x')\} \quad (5.11)$$

from (5.3) and (5.10), we obtain for \mathcal{L}_A

$$K_{AB}^{(1)}(x-x') = i(\Gamma_\mu \partial_\mu \tau_\nu \epsilon_{;\nu} - m e^{-i\alpha \Gamma_5})_{AB} \Delta(x-x') \quad (5.12)$$

and for \mathcal{L}_B

$$K_{AB}^{(2)}(x-x') = -i\epsilon \{\Gamma_5 \Gamma_\mu \partial_\mu \tau_\nu \epsilon'_{;\nu} - m e^{-i\beta \Gamma_5} (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau}\}_{AB} \Delta(x-x') \quad (5.13)$$

With

$$\begin{aligned} \Delta(x-x') &= -\Delta(x'-x) \\ \frac{\partial \Delta(x-x')}{\partial x} &= \frac{\partial \Delta(x'-x)}{\partial x'} \end{aligned} \quad (5.14)$$

the supplementary condition for Φ gives the following identity

$$K(x-x') \equiv AK^T(x'-x)A \quad (5.15)$$

where A is defined by help of formula (4.1).

After substitution of (5.12-13) in (5.15) we get

$$K^{(1)} \equiv -K^{(1)} \quad K^{(2)} \equiv K^{(2)} \quad (5.16)$$

for arbitrary isotensors in $K^{(1)}$ and $K^{(2)}$.

It may be easily seen from (5.16) that the Lagrangian \mathcal{L}_B is the true Lagrangian of our quantized equation, if from the two possibilities in (5.3) and according to (5.11) the anti-commutators are chosen.

For commutators we obtain instead of (5.15)

$$K(x-x') \equiv -AK^T(x'-x)A \quad (5.17)$$

and the Lagrangian \mathcal{L}_A describes boson fields, satisfying our generalized Dirac equation⁴.

The relation (5.13) fully determines the commutation relations between $\Psi_{\alpha;\beta}$ and $\Psi_{\gamma;\delta}^+$. Let us introduce

$$\phi^{(\pm)} = P^{(\pm)}\phi \quad (5.18)$$

where, assuming

$$(P^{(\pm)})^2 = P^{(\pm)} \quad (5.19a)$$

$$P^{(+)}P^{(-)} = P^{(-)}P^{(+)} = 0 \quad (5.19b)$$

⁴ The problem of "spinor-bosons" satisfying the Dirac equation will be investigated elsewhere.

we may put for $\epsilon = -1$

$$P^{(\pm)} = \frac{1}{2} \left(1 \pm \frac{(i\Gamma_5 \vec{E} + \vec{D})\vec{\tau}}{\sqrt{D^2 - E^2}} \right) \quad (5.20)$$

The subsidiary condition implies

$$\Phi^{(+)} = \hat{A}\Phi^{(-)} = A\overline{\Phi^{(-)}} \quad (5.21)$$

Thus from both 8-spinors (5.18), we shall take into account only the 8-spinor $\Phi^{(+)}$. Using

$$\overline{\Phi^{(\pm)}} = (P^{(\pm)})^T \overline{\Phi} \quad (5.22)$$

we obtain

$$\{\Phi_A^{(+)}, \Phi_B^{(+)}\} = (P^{(+)}K^{(2)}P^{(-)}A^T)_{AB} \quad (5.23)$$

and because

$$[P^{(\pm)}, K^{(2)}] = 0 \quad (5.24)$$

from (5.19b) we have

$$\{\Phi_A^{(+)}, \Phi_B^{(+)}\} = 0 \quad (5.25)$$

Similarly

$$\{\overline{\Phi_A^{(+)}}, \overline{\Phi_B^{(+)}}\} = 0 \quad (5.26)$$

Using (5.22) it is easy to show that

$$\{\overline{\Phi_A^{(+)}}, \Phi_B^{(+)}\} = (P^{(+)}K^{(2)}P^{(+)})_{AB} \quad (5.27)$$

or, by virtue of (5.19a) and (5.24)

$$\{\overline{\Phi_A^{(+)}}, \Phi_B^{(+)}\} = (P^{(+)}K^{(2)})_{AB} \quad (5.28)$$

Calculating (5.28), as

$$(i\Gamma_5 \vec{E} + \vec{D})\vec{\tau} \cdot P^{(\pm)} = \pm \sqrt{D^2 - E^2} \cdot P^{(\pm)} \quad (5.29)$$

we get finally

$$\{\overline{\Phi_A^{(+)}}, \Phi_B^{(+)}\} = \frac{i}{2} \{[\sqrt{D^2 - E^2} + (i\Gamma_5 \vec{E} + \vec{D})\vec{\tau}] \cdot (\Gamma_\mu \partial_\mu \tau_\nu \epsilon_{;\nu} - me^{-i\beta\Gamma_5})\}_{AB} \cdot \Delta(x - x^2)$$

where $\epsilon_{;\nu}$ is a unit isovector parallel to $\kappa_{;\nu}$.

6. The Jauch Field

The field which obeys the commutation relations (0.5) was first proposed by Jauch in 1954.

We introduce the transformation

$$\Phi \rightarrow \Phi^B = B\Phi \quad (6.1)$$

which transforms (0.5) in the conventional anticommutation relations for the Dirac field, namely

$$\begin{aligned}\{\bar{\psi}_\alpha(x), \psi_\beta(x')\} &= -iS_{\alpha\beta}(x-x') \\ \{\hat{\psi}_\alpha(x), \psi_\beta(x')\} &= 0\end{aligned}\quad (6.2)$$

Let us insert the Majorana representation of the γ_μ -matrices (Majorana 1937), for which

$$\psi^c \equiv C\bar{\psi} = \psi^+ \quad (6.3)$$

We have

$$\Phi = \frac{1}{\sqrt{2}} \left(\frac{\psi}{\gamma_5 \psi^+} \right) \quad \bar{\Phi} = \frac{1}{\sqrt{2}} (\bar{\psi}_1 - \bar{\psi} \gamma_5) \quad (6.4)$$

The commutation relations (0.5) can be written by help of (6.4)

$$K_{AB}^{(I)}(x-x') = -i\{(\tau_3 - i\Gamma_5 \tau_2 \varrho)(\Gamma_\mu \partial_\mu \tau_3 - m)\}_{AB} \cdot \Delta(x-x') \quad (6.5)$$

and similarly (6.2)

$$K_{AB}^{(D)}(x-x') = -i\{\tau_3(\Gamma_\mu \partial_\mu \tau_3 - m)\}_{AB} \cdot \Delta(x-x') \quad (6.6)$$

Putting in (6.1)

$$B = \exp \left(-\tau_1 \Gamma_5 \frac{\beta}{2} \right) \quad (6.7)$$

we obtain from (6.6)

$$B^{-1} K_{AB}^{(D)}(x-x') B = \exp(\tau_1 \Gamma_5 \beta) \cdot K_{AB}^{(D)}(x-x') \quad (6.8)$$

Because

$$\exp(\tau_1 \Gamma_5 \beta) \cdot \tau_3 = \frac{1}{1-\varrho^2} (\tau_3 - i\Gamma_5 \tau_2 \varrho) \quad (6.9)$$

if

$$\cosh \beta = \frac{1}{1-\varrho^2} \quad (6.10)$$

after the scale transformation

$$\Phi \rightarrow \frac{1}{\sqrt{1-\varrho^2}} \Phi \quad (6.11)$$

we obtain from the Dirac commutation relations (6.2) the Jauch commutation relations (0.5), where the transformation (5.7) is an isorotation in the (1,4)-isoplane.

The transformation (6.7) do not change the isovector $\kappa_{;\mu}$, chosen for the Dirac and Jauch fields by means of (0.1).

The full 3-parameter group, which leaves the mass isovector components (0.1) invariant, is

$$\psi' = a\psi + b\psi^c \quad |a|^2 - |b|^2 = 1 \quad (6.12a)$$

or, using 8-spinor notation,

$$\Phi' = \exp \left\{ -\frac{1}{2} (\varrho_1 \tau_1 + \varrho_2 \tau_2) \Gamma_5 + \frac{i}{2} \alpha \tau_3 \right\} \cdot \Phi \quad (6.12b)$$

It may be divided into two subgroups \mathcal{Q} and \mathbf{J} :

$$\mathcal{Q}: \quad \Phi' = \exp \left(\frac{i}{2} \alpha \tau_3 \right) \Phi \quad (6.13)$$

$$\mathbf{J}: \quad \Phi' = \exp \left\{ -\frac{1}{2} (\varrho_1 \tau_1 + \varrho_2 \tau_2) \Gamma_5 \right\} \Phi \quad (6.14)$$

The 1-parameter group \mathcal{Q} leaves the free antisymmetrized Schwinger Lagrangian (Schwinger 1948) invariant:

$$\mathcal{L}_0 = \frac{1}{2} \bar{\psi} (\gamma_\mu \partial_\mu + m) \psi + \frac{1}{2} \bar{\psi}^c (\gamma_\mu \partial_\mu + m) \psi^c \quad (6.15a)$$

or, using 8-spinors as in Sect. 4,

$$\mathcal{L}_0 = \bar{\Phi} \tau_3 (\Gamma_\mu \partial_\mu \tau_3 + m) \Phi \quad (6.15b)$$

\mathcal{Q} can be used as an electric charge gauge-transformation group, not changing the Lagrangian and the conventional commutation relations (6.2).

The 2-parameter group \mathbf{J} leads to a generalized Jauch field, described by the commutation relations (0.5), (0.5b). If we transform (5.6) by means of (6.14), we obtain after a scale transformation

$$\Phi \rightarrow \frac{1}{\sqrt{1 - \varrho_1^2 - \varrho_2^2}} \Phi \quad (6.16)$$

that in (0.5b)

$$\varrho = \varrho_1 + i\varrho_2 \quad (6.17)$$

The Jauch field differs from the Dirac field only by another choice of the commutation relations. Thus we see that in quantum theory a 4-spinor field is not determined by the equation uniquely.

7. The Second Isovector $\epsilon'_{;\mu}$

By (4.15), (4.8) and (5.6-7) we have (for $\beta=0$)

$$\mathcal{L}_0 = \bar{\Phi} (i\Gamma_5 \vec{E} + \vec{D}) \vec{\tau} \cdot (\Gamma_\mu \partial_\mu \tau_\nu \epsilon_{;\nu} + m) \Phi \quad (7.1)$$

where

$$\epsilon_{;\nu} = \frac{\varkappa_{;\nu}}{m} \quad (7.1a)$$

The Lagrangian (6.15) of Schwinger is obtained from (7.1) by putting (0.1) and

$$\vec{E} = 0 \quad \vec{D} = (0, 0, 1) \quad (7.2)$$

It is easily seen that (6.15) transforms under (6.7) to the following Lagrangian of Jauch field:

$$\mathcal{L}_0 = \Phi(\tau_3 + i\Gamma_5 \varrho \tau_2)(\Gamma_\mu \partial_\mu \tau_3 + m)\Phi \quad (7.3)$$

Using (4.8) and (4.11) we have

$$\vec{E} = (0, \varrho, 0) \quad \vec{D} = (0, 0, 1) \quad (7.3a)$$

From (7.1) it may be seen that the Lagrangian of our generalized field is determined by the choice of $\epsilon_{;v}$ and $E_{;\mu\nu} = (\vec{E}, \vec{D})$, or, taking into account (4.8), by the choice of $\epsilon'_{;v}$ and $E_{;\mu\nu}$.

Let us consider the connexion between $\epsilon_{;v}$, $\epsilon'_{;v}$ and $E_{;\mu\nu}$. Using (3.22a), (3.20a) and (3.21), we obtain

$$\kappa_{;v} = -|b|\epsilon'_{;\mu}E_{;\mu\nu} \quad (7.4)$$

and

$$\epsilon_{;v} = C \cdot \epsilon'_{;\mu}E_{;\mu\nu}, \quad (7.5)$$

where

$$C = -\frac{|b|}{m} \quad (7.5a)$$

From antisymmetry of $E_{;\nu\mu}$ we obtain the relation

$$\epsilon_{;v}\epsilon'_{;v} = C \cdot \epsilon'_{;\mu}E_{;\mu\nu}\epsilon'_{;v} = 0 \quad (7.6)$$

which by virtue of (7.1) is equivalent to (0.2). Therefore, $\epsilon_{;\mu}$ and $\epsilon'_{;\mu}$ are orthogonal. As it is proved in Appendix I that

$$\epsilon_{;\mu}\check{E}_{;\mu\nu} = 0, \quad (7.7)$$

the isovector $\epsilon_{;\mu}$ is orthogonal to the isoplane described by the isotensor $\check{E}_{;\mu\nu}$.

It is necessary to mention that if the invariant $E_{;\mu\nu}\check{E}_{;\mu\nu}$ vanish, $E_{;\mu\nu}$ and $\check{E}_{;\mu\nu}$ describe two orthogonal isoplanes. Because for each isoplane in 4-dimensional space, there is only one orthogonal isoplane, we see from (3.16), (3.21) and (7.7) that $\epsilon_{;\mu}$ and $\epsilon'_{;\mu}$ are parallel to the isoplane described by $E_{;\mu\nu}$. Taking into account the identity (7.6), we conclude that the isovectors $\epsilon_{;\mu}$ and $\epsilon'_{;\mu}$ (or $\kappa_{;\mu}$ and $\epsilon'_{;\mu}$) describe a 2-dimensional orthogonal coordinate system on this isoplane.

Comparing (6.15) and (4.8), we obtain for $\epsilon'_{;\mu}$ in Schwinger's case the relation (0.3), and in Jauch's case — (0.4).

The isoplane, orthogonal to $\epsilon_{;\mu}$ and $\epsilon'_{;\mu}$ (described by means of $\check{E}_{;\mu\nu}$) is the electric charge isoplane. In Schwinger's case it is, in accordance with (0.1) and (0.3), the (1.2)-isoplane. The rotations in the electric charge isoplane describe, in accordance with (6.13), the electric charge gauge-group \mathcal{Q} .

8. Conclusions

The theory is determined by a pair of orthogonal isovectors in Minkowski's isospace. Because (see (3.8), (7.1a)) always $\epsilon_{;\mu}^2 > 0$, we have the following two invariants with respect to the C' -rotation classes of the Lagrangians:

$$\epsilon_{;\mu}^2 = 1 \quad \epsilon'_{;\mu}{}^2 = -1 \quad (8.1)$$

euclidean electric charge isoplane
and

$$\epsilon_{;\mu}^2 = 1 \quad \epsilon'_{;\mu}{}^2 = +1 \quad (8.2)$$

(pseudoeuclidean electric charge isoplane).

The Dirac-Schwinger choice (0.1)–(0.3) belongs to (8.1).

It may be shown that we pass from type (8.1) to type (8.2) after, e.g., by the following interchange of the Lagrangian (6.15b):

$$\mathcal{L}_0 = i\bar{\Phi}\Gamma_5\tau_2(\Gamma_\mu\partial_\mu\tau_3 + m)\Phi \quad (8.3)$$

which leads to the commutation relations

$$\begin{aligned} \{\bar{\psi}_\alpha(x), \psi_\beta(x')\} &= 0 \\ \{\hat{\psi}_\alpha(x), \psi_\beta(x')\} &= -iS_{\alpha\beta}(x-x')\Delta(x-x') \end{aligned} \quad (8.4)$$

Both cases (8.1) and (8.2) admit the introduction of the following generalized commutation relations

$$\begin{aligned} \{\bar{\psi}_\alpha(x), \psi_\beta(x')\} &= \alpha S_{\alpha\beta}(x-x')\Delta(x-x') \\ \{\hat{\psi}_\alpha(x), \psi_\beta(x')\} &= \beta S_{\alpha\beta}(x-x')\Delta(x-x') \end{aligned} \quad (8.5)$$

where α, β are complex and

$$\alpha \neq \beta \quad (8.5a)$$

The form (8.5) of the most general commutation relations is written for the choice (0.1) of the mass-isovector components.

9. Final Remarks

In this paper the quantum theory of 4-spinor fields, invariant with respect to $C \times C'$ is developed. From our point of view, it may be interesting to discuss the following two problems:

1) The connection of the 4-spinor theory with the 8-spinor theory, which describes, as we suppose, the free baryon field. It may be mentioned that the supplementary condition

$$\Phi \equiv \hat{A}\Phi \quad (9.1)$$

can be treated as a baryonic number neutrality condition.

2) The introduction of the interaction Lagrangians, invariant with respect to $C \times C'$. We intend to investigate further these problems elsewhere.

The author would like to thank Professor Rzewuski for his advices and many, helpful discussions.

APPENDIX I

If a certain isovector $\epsilon'_{3\mu}$ exists, which satisfies (3.21), then the mixed invariant obtained from the two isotensors $E_{3\mu\nu}$, $\check{E}_{3\mu\nu}$ vanishes identically. This theorem may be simply proved by obtaining first the result that the isotensor

$$G_{3\mu\nu} = E_{3\mu\varrho} \check{E}_{3\varrho\nu} \quad (\text{A.1})$$

is diagonal.

Indeed, the relation (A.1) can be written

$$G_{3\mu\nu} = \frac{1}{2i} E_{3\mu\varrho} \epsilon_{\nu\varrho\tau\sigma} E_{3\tau\sigma} \quad (\text{A.2})$$

Let us assume $\mu \neq \nu$. Thus, if $\varrho_1 \neq \varrho_2$ and $\mu \neq \varrho_1 \neq \nu$, $\mu \neq \varrho_2 \neq \nu$, the isotensor component (A.2) is equal to the following sum of four terms⁵

$$G_{3\mu\nu} = \frac{1}{2i} \{ E_{3\mu\varrho_1} \epsilon_{\nu\varrho_1\varrho_2\mu} E_{3\varrho_2\mu} + E_{3\mu\varrho_2} \epsilon_{\nu\varrho_2\varrho_1\mu} E_{3\varrho_1\mu} \} + \frac{1}{2i} \{ E_{3\mu\varrho_1} \epsilon_{\nu\varrho_1\mu\varrho_2} \times \\ \times E_{3\mu\varrho_2} + E_{3\mu\varrho_2} \epsilon_{\nu\varrho_2\mu\varrho_1} E_{3\mu\varrho_1} \} \quad (\text{A.3})$$

Using the antisymmetry property of $E_{3\mu\nu}$ and $\epsilon_{\mu\nu\tau\varrho}$, we obtain the result that the first term in (A.3) is equal to the second, and similarly, the third to the fourth. We have

$$G_{3\mu\nu} = 0 \quad \mu \neq \nu \quad (\text{A.4})$$

and

$$G_{3\mu\nu} = t_{3\mu} \cdot \delta_{3\mu\nu} \quad (!) \quad (\text{A.5})$$

The form (A.5) is not invariant under C' -isorotations. Thus

$$t_{3\mu} = t = \frac{1}{4} \text{Sp } G_{3\mu\nu} \quad (\text{A.6})$$

Because

$$\text{Sp } G_{3\mu\nu} = - E_{3\mu\varrho} \check{E}_{3\mu\varrho} \quad (\text{A.7})$$

we have

$$G_{3\mu\nu} = - \frac{1}{4} E_{3\lambda\varrho} \check{E}_{3\lambda\varrho} \delta_{3\mu\nu} \quad (\text{A.8})$$

From (A.8) we obtain

$$G_{3\mu\nu} = G_{3\nu\mu} \quad (\text{A.9})$$

⁵ We do not use here the Einstein summation convention.

and, using (3.21)

$$\epsilon'_{;\mu} G_{;\mu\nu} = \epsilon'_{;\mu} G_{;\nu\mu} = \epsilon'_{;\mu} \check{E}_{;\mu\varrho} E_{;\varrho\nu} = 0 \quad (\text{A.10})$$

On the other hand, it follows from (A.8) that

$$\epsilon'_{;\mu} G_{;\mu\nu} = -\frac{1}{4} E_{;\lambda\varrho} \check{E}_{;\lambda\varrho} \epsilon'_{;\nu} \quad (\text{A.11})$$

and, if such a ν exists for which $\epsilon'_{;\nu} \neq 0$, we obtain (3.16). Now we show the validity of (7.7). Using (7.5) and (A.9), we get

$$\begin{aligned} \epsilon_{;\varrho} \check{E}_{;\varrho\nu} &= C \cdot \epsilon'_{;\mu} E_{;\mu\varrho} \check{E}_{;\varrho\nu} = C \cdot \epsilon'_{;\mu} G_{;\mu\nu} = C \cdot \epsilon'_{;\mu} G_{;\nu\mu} \\ &= C \cdot \epsilon'_{;\mu} E_{;\nu\varrho} \check{E}_{;\varrho\mu} = C \cdot \epsilon'_{;\mu} \check{E}_{;\mu\varrho} \cdot E_{;\nu\varrho} \end{aligned} \quad (\text{A.12})$$

and if relation (3.21) is valid, the right side of (A.12) vanishes and relation (7.7) is proved.

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MEASUREMENT OF THE MEAN LIFE OF THE FIRST EXCITED STATE OF Ne^{23}

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The mean life of the first excited state on Ne^{23} was measured using resonance fluorescence technique. Ne^{23} obtained from $\text{Ne}^{22}(\text{n}, \gamma)\text{Ne}^{23}$ reaction by irradiation neon in the reactor was used as a source. The value of the mean life was found to be $\tau = (1.5 \pm_{-0.2}^{+0.3}) \times 10^{-12}$ sec.

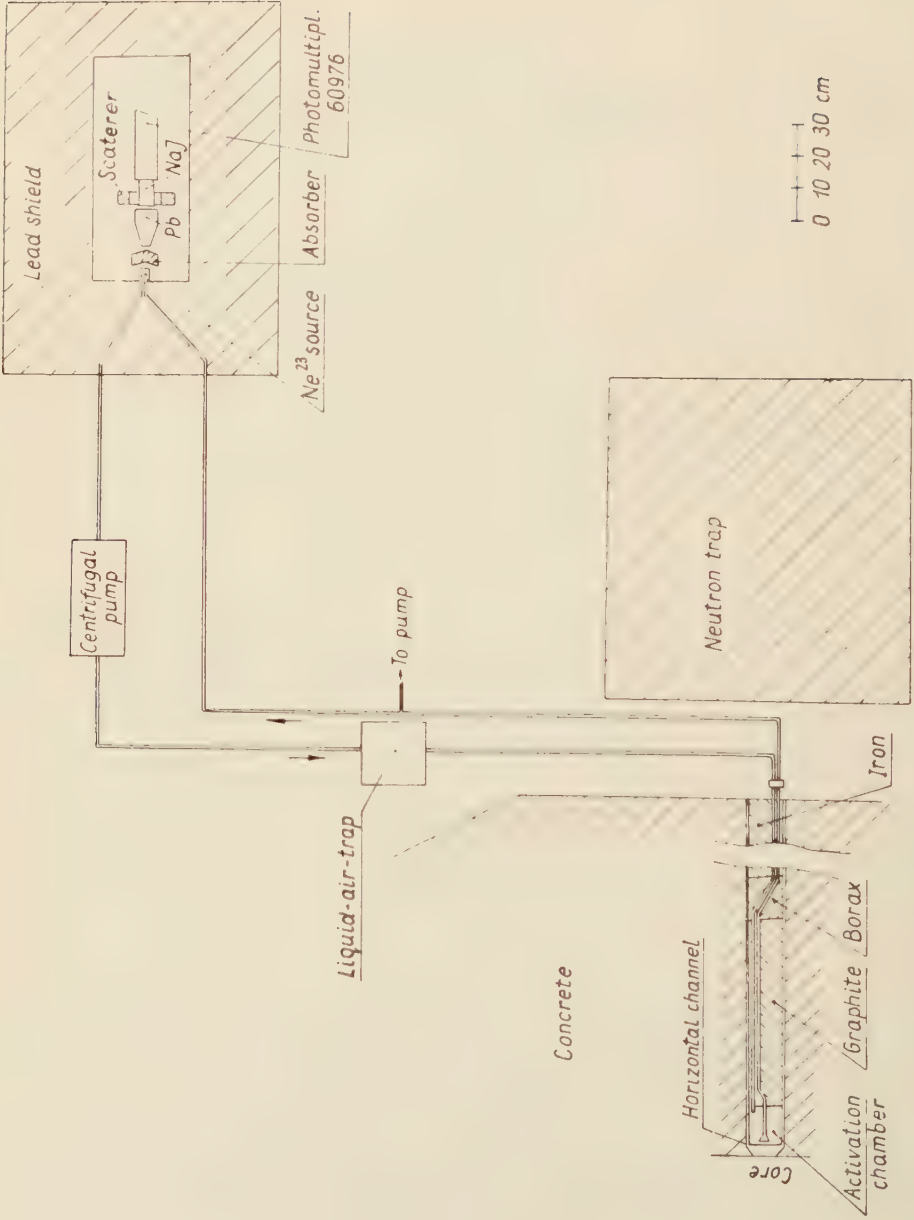
1. Introduction

In view of the possibility of obtaining information on β - ν angular correlations by using nuclear fluorescence technique [1], [2], we have undertaken the investigation of the decay of Ne^{23} , which is a suitable isotope for this purpose, as suggested by Lewis and Curtis [2]. There is a marked discrepancy between the results of measurements of the mean life of the first excited state of Ne^{23} published by various authors: Booth *et al.* $\tau = (1.5 \pm 0.3) \times 10^{-10}$ sec [3], Krone *et al.* $\tau = 10^{-12} - 10^{-13}$ sec [4], Rasmussen *et al.* $\tau = (1.8 \pm_{-0.3}^{+0.4}) \times 10^{-12}$ sec [5]. Therefore we have undertaken to measure this mean life once more applying the self-absorption method [6], [7].

Results concerning the decay scheme of Ne^{23} will be published separately.

2. Experimental

The experimental arrangement is shown in fig. 1. Ne^{23} was obtained from the $\text{Ne}^{22}(\text{n}, \gamma)\text{Ne}^{23}$ reaction by irradiation of spectrally pure Ne in the reactor "EWA". The thermal neutron flux around the activation chamber was $10^{12} \frac{n}{\text{cm}^2 \text{ sec}}$. The gas was circulated by a centrifugal pump driven by an electric motor. The voltage on the motor was stabilized. Since the intensity was dependent on the pumping speed, care was taken to work in an interval where this dependence is approximately flat. Therefore the intensity of the Ne^{23} source was constant within 1%. The brass source chamber had a cylindrical shape and dimensions: $\varnothing 30 \times 40$ mm and wall thickness 1 mm. The possible source inhomogeneity did not exceed 5% along the axis. The source intensity during the measurements was about $100 \mu\text{C}$.



0 10 20 30 cm

Fig. 1

A $2'' \times 2''$ NaJ(Tl) crystal mounted on EMI 6097B phototube was used. The pulses were analysed by a 100 channel pulse height analyser. The half width of the spectrometer was 12% for 661 keV line of Cs^{137} .

As the source intensity was small a thick scatterer had to be used. The sodium scatterer and absorber were prepared in thin wall plexiglass containers by melting the sodium in vacuum. The thickness of the absorber was 4 cm. The dimensions of the scatterers were as follows: $\Phi_{\text{ext}} = 15.5$ cm, $\Phi_{\text{int}} = 7.5$ cm, thickness 4.0 cm. The comparison scatterer was made of crushed metallic magnesium, the comparison absorber of aluminium plates. The dimensions of the comparison scatterer and absorber were the same, as those of the sodium. In order to match both scatterers for Compton scattering and pair production, a small amount of paraffin was added to the magnesium scatterer. The matching of the scatterers was checked with Au^{198} and Pr^{142} sources. The absorbers were checked by comparison of the attenuation of the intensity of the Compton scattered γ -rays from the magnesium scatterer. The relative sensitivity of the NaJ(Tl) crystal for different points of the scatterer was measured using Au^{198} .

3. Results

The measurements were made in the neighbourhood of the reactor. Sometimes, in spite of thick asphalt-lead shields, some fluctuations of the background, in intensity and shape of energy spectrum, were observed during the measurements. It was established that this fluctuations with good approximation could be considered as linear *vs* energy in the resonance region. Taking this into account the spectra obtained with the sodium scatterer were normalized to this obtained with the magnesium scatterer. The corresponding curves obtained in this way are shown in fig. 2. The rather large background in the 440 keV region is caused by the high energy part of the γ -radiation near the reactor.

Fig. 3 shows the difference curves obtained by subtraction of the spectrum measured with the magnesium scatterer and aluminium absorbers. The fluctuations of experimental points at the left edge of each spectrum are predominantly statistical in origin (partially they would be caused by random errors in the placement of the scatterers). In the normalization procedure, mentioned above, both spectra have been cut off along a straight line connecting their right edge and the valley between the compton edge and the photo-peak. This is why the spectra are asymmetric and they go to zero at the left edge. The shapes of the spectra marked out by the experimental points are consistent with the shape of the 440 keV line of Ne^{23} .

The measured intensity ratio (see appendix) is $\frac{s}{s_0} = 0.51 \pm 0.04$. Using the equation 2 of the appendix, with $T_{\text{ef}} = 305^\circ$ [8], [9], $I_0 = \frac{3}{2}$; $I_1 = \frac{5}{2}$ [10], [11], [12], [13] we obtain $K = 0.27 \pm 0.045$. From this the mean life was found to be $\tau = (1.5^{+0.3}_{-0.2}) \times 10^{-12}$ sec.

This is in disagreement with the result obtained by Booth *et al.* [3] in a similar experiment as ours and in good agreement with that obtained recently by Rasmussen *et al.* [5], who used the 440 KeV γ -radiation from Na^{23} (p, p'). From their results $\tau = (1.8^{+0.4}_{-0.3}) \times 10^{-12}$ and the known partial lifetime for electric quadrupole transition ($E2$) $= 5.6 \times 10^{-10}$ sec. [14], [15],

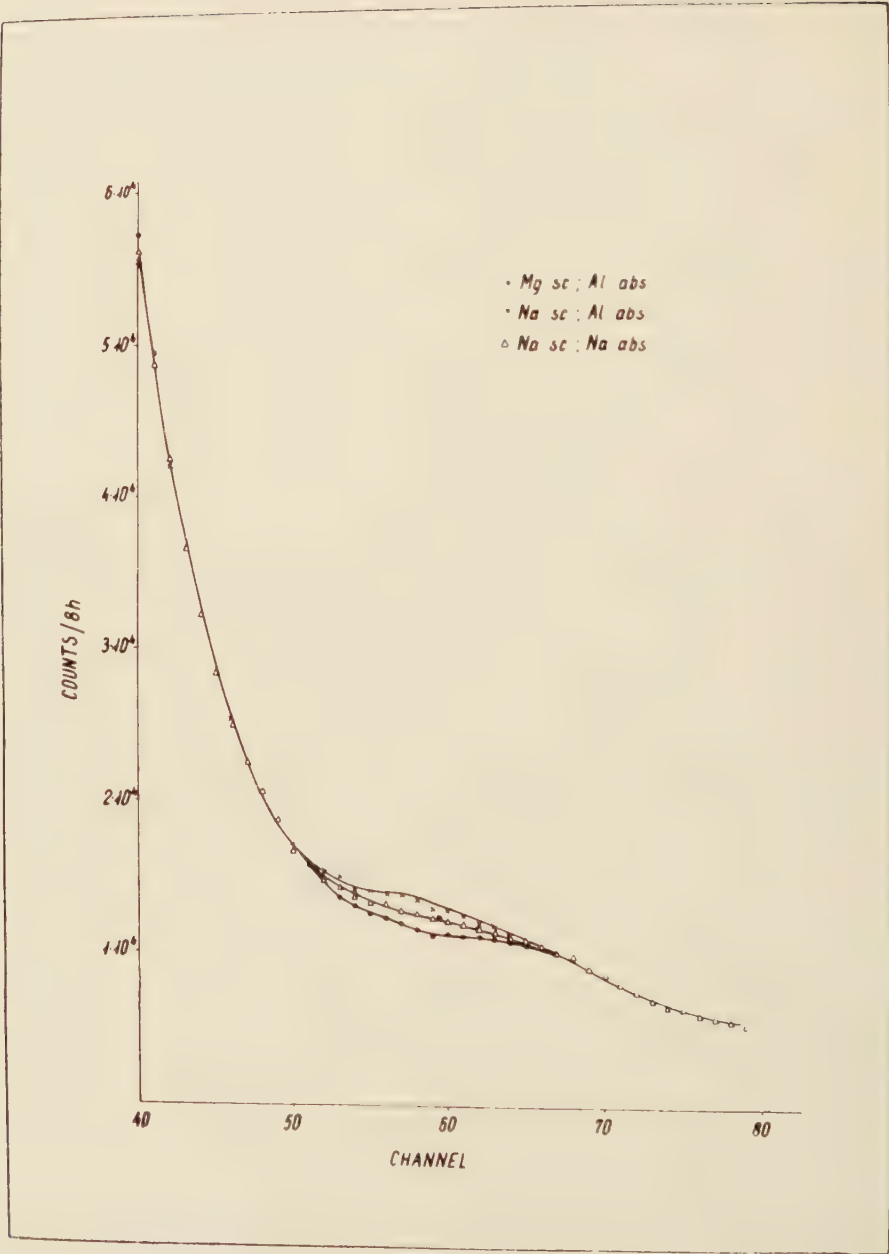


Fig. 2

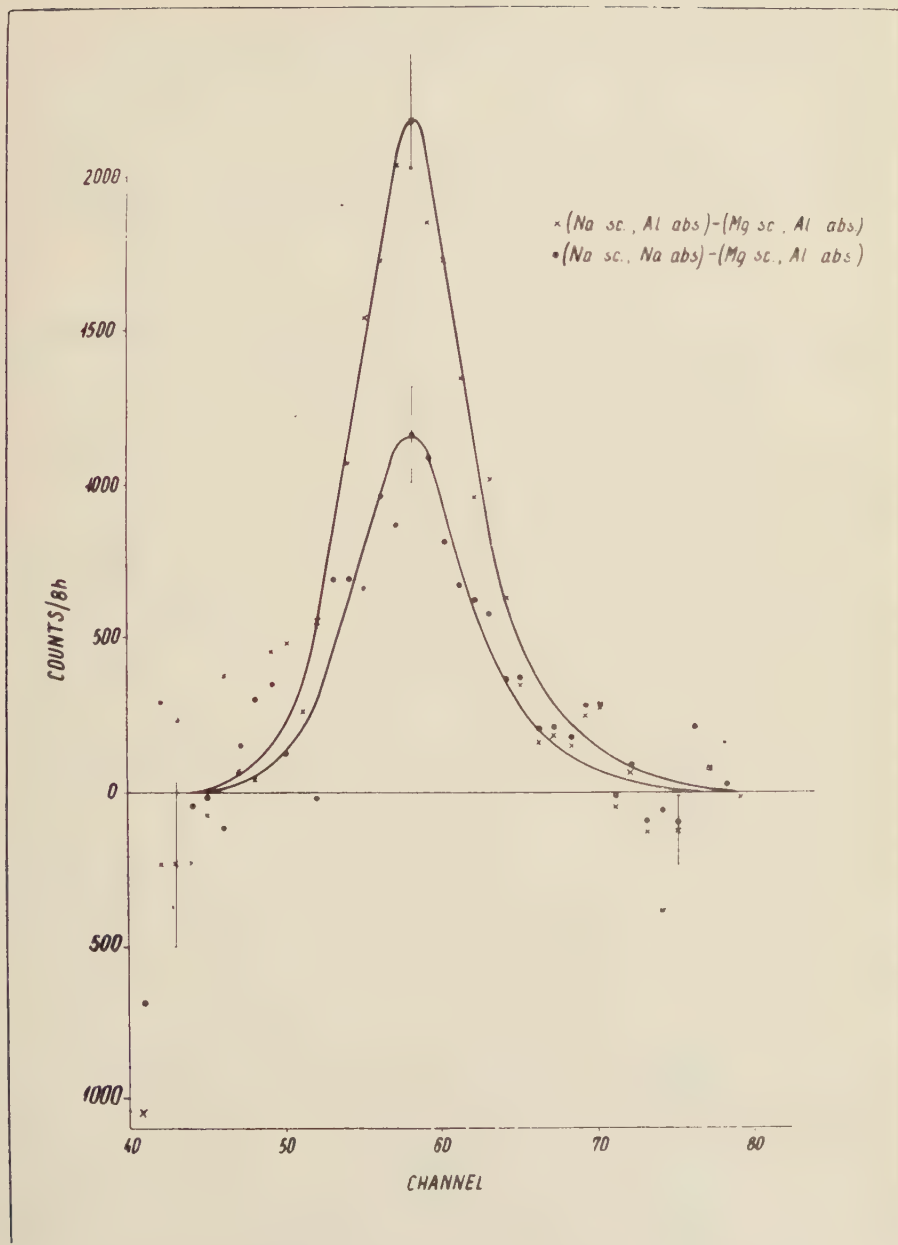


Fig. 3

[16], they found the $\frac{E2}{M1}$ amplitude ratio $\delta = 0.056$ and from angular distribution of resonantly scattered γ -rays they found δ to be rather positive.

The mean life calculated from the unified model [17] and from the single — particle Weisskopf formula (for M1 transition) is 4×10^{-13} sec, which is not too far from the experimental value.

The authors would like to thank Dr Z. Wilhelmi, chief of Nuclear Physics Laboratory, for the kind interest shown in the present measurements, Mgr Eng. J. Aleksandrowicz and all members of reactor crew for many facilities in performing of the measurements.

APPENDIX

Taking into account the geometry shown in fig. 4 it is seen that the number of counts of resonantly scattered (assuming isotropy) γ -rays is given by.

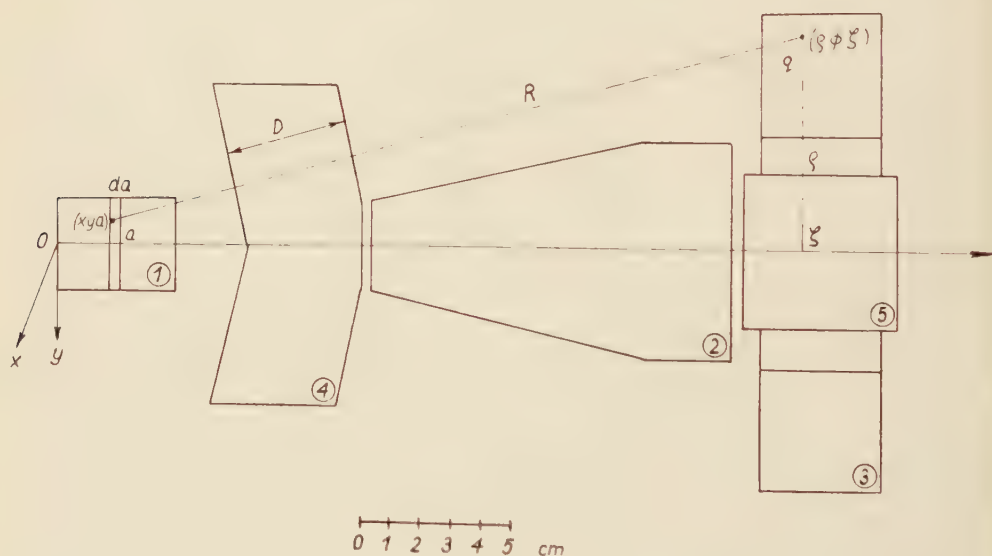


Fig. 4

$$S(D, K) = \text{const} \int \frac{d\tau_1 d\tau_2}{R^2} \varepsilon(\zeta, \varrho) e^{-\mu q} F(D + q, K) \quad (1)$$

where

$$d\tau_1 = dx dy da$$

$$d\tau_2 = \varrho d\varrho d\zeta d\Phi$$

$$F(q, K)^1 = \sum_{m=0}^{\infty} \frac{(-Kq)^m}{m! (m+1)^{1/2}}$$

¹ $F(q, K)$ was tabulated by S. Ofer and A. Schwarzschild [7].

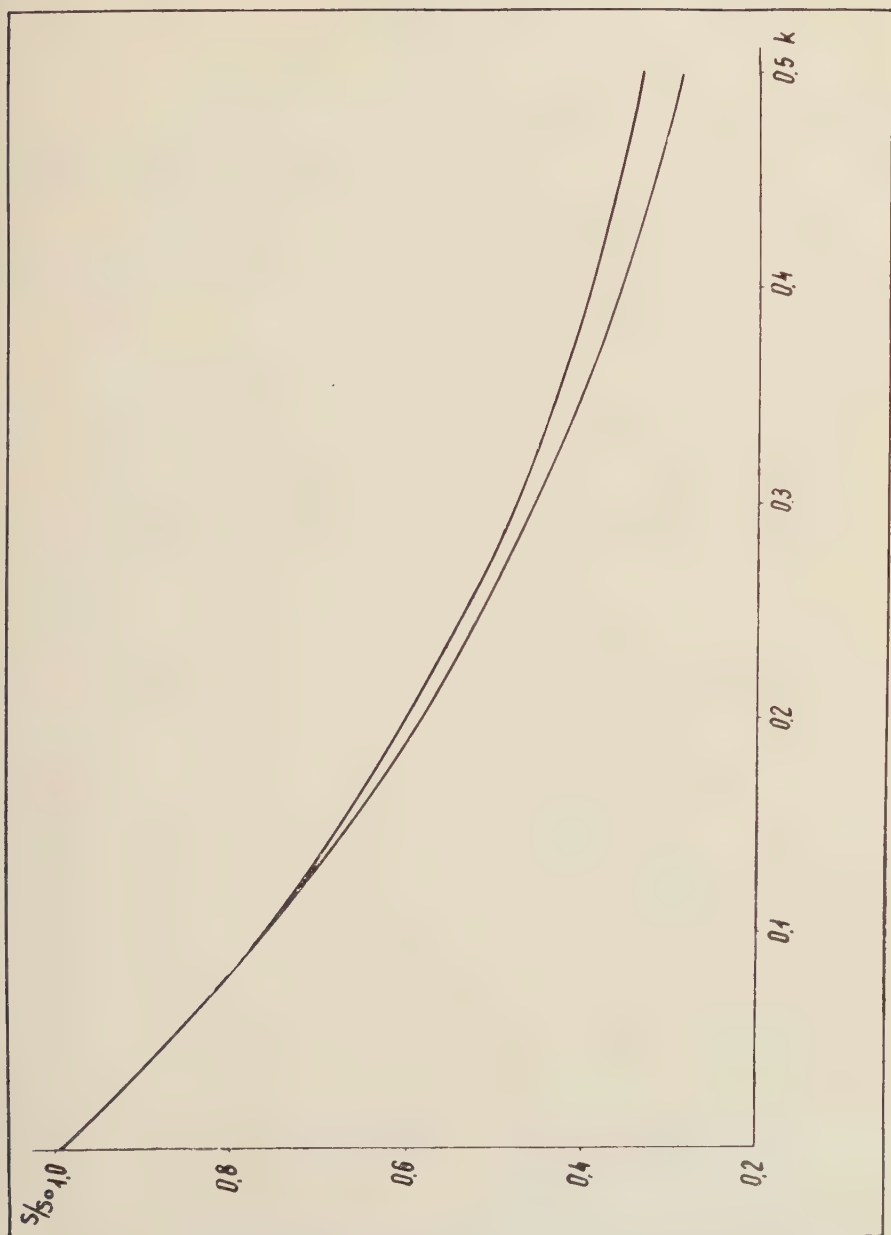


Fig. 5

$$K = n\pi^{3/2} \tilde{\chi}^2 \frac{2I_1 + 1}{2I_0 + 1} \frac{I}{J}$$

$$A = E_r \left(\frac{2K T_{\text{ef}}}{Mc^2} \right)^{1/2}$$

T_{ef} is the effective temperature of the sodium scatterer and absorber.

n is the number of sodium nuclei per cm^3

$\varepsilon(\tilde{\zeta}, \varrho)$ is the relative sensitivity of the NaJ(Tl) crystal for various parts at the scatterer

$\varepsilon(\tilde{\zeta}, \varrho) = \varepsilon'(\tilde{\zeta}, \varrho) e^{-\mu' \varrho} e^{-\mu \varrho}$. $\varepsilon'(\tilde{\zeta}, \varrho)$ was measured experimentally when the scatterer was removed.

μ is the total nonresonance absorption coefficient of the scattering material.

If we put in formula (1) instead of $q = q(x, y, a, \tilde{\zeta}, \varrho)$ and $R = R(x, y, a, \tilde{\zeta}, \varrho)$ the values $\bar{q} = \bar{q}(\bar{x}, y, a, \tilde{\zeta}, \varrho)$, $\bar{R} = \bar{R}(\bar{x}, y, a, \tilde{\zeta}, \varrho)$ averaged over x and y , which is a good approximation for our geometry, we obtain by integrating over Φ

$$\frac{S}{S_0} = \frac{S(D, K)}{S(O, K)} = \frac{\int da d\tilde{\zeta} d\varrho \frac{\varrho}{R^2} \varepsilon(\tilde{\zeta}, \varrho) F(D + q, K) e^{-\mu q} S_a(\tilde{\zeta}, \varrho)}{f(D = 0)} \quad (2)$$

S_a is the cross section surface (for a given fixed a) of the source chamber seen from the point

$(\tilde{\zeta}, \varrho)$ of the scatterer. The curve $\frac{S}{S_0}$ vs K numerically calculated from equation (2) for our

geometry is shown in fig. 5. For comparison $\frac{S}{S_0} = F(D, K)$ for the case of a thin scatterer is also plotted (the lower curve).

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ÜBER DIE QUANTENTHEORIE DER ANTIFERRIMAGNETIKA

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Es wird mit Hilfe der Methode von Holstein-Primakoff die Dispersionsformel für Ferrite mit einer inversen Spinellstruktur berechnet. Wegen der magnetischen Überstruktur erhält man eine anisotrope Dispersionsformel. Im Falle gleich grosser Spins bei den Oktaeder-Gitterplätzen ist für Antiferrimagnetika $E \sim K^2$. Es wird gezeigt, dass die Ergebnisse der korrigierten Arbeiten von Wonsowski und Seidow und von Kondorski, Pachomow und Siklós sich gleichwertig sind und mit den Ergebnissen der vorliegenden Arbeit übereinstimmen.

I. Einleitung

In der letzten Zeit erschien eine Reihe von Theoretischen Arbeiten (z.B.: Wonsowski u. Seidow 1954; Kondorski und seine Mitarbeiter 1957; Kaplan 1958) über antiferrimagnetische Körper mit einer Spinellstruktur. Das Wesentliche dieser Struktur ist ein aus Sauerstoff-Ionen O^{2-} gebildetes, kubisch-flächenzentriertes Gitter, in das die Metall-Ionen Me^{++} , Fe^{+++} eingebettet sind, wobei sie Tetraeder-Zwischenräume (A), beziehungsweise Oktaeder-Zwischenräume (B) einnehmen. Es wird vorausgesetzt, dass die dreiwertigen Eisen-Ionen in den Zwischenräumen (A) einen Gesamtspin σ , die dreiwertigen Eisen-Ionen in den Zwischenräumen (B) den Spin S und die zweiwertigen Metall-Ionen in den Zwischenräumen (B) den Spin s besitzen.

Die Rolle der Sauerstoff-Ionen in der Wechselwirkung zwischen den magnetischen Ionen berücksichtigen wir, indem wir Superaustauschintegrale einführen.

Die Ergebnisse der oben erwähnten Arbeiten widersprechen sich gegenseitig. Die von Wonsowski u. Seidow (1954) abgeleitete Dispersionsformel für Spinwellen besteht aus zwei Energiezweigen (E) die beide linear von der Wellenzahl K abhängen, wenn man nur die Wechselwirkung zwischen den (A) und (B) Ionen berücksichtigt (die $A-A$ und $B-B$ Wechselwirkungen sind verschwindend klein im Vergleich mit der $A-B$ Wechselwirkung). Die Dispersionsformel aus der Arbeit von Kondorski und seinen Mitarbeitern (1957) besteht gleichfalls aus zwei Zweigen, die beide vom Quadrat der Wellenzahl abhängen. Sowohl Wonsowski u. Seidow als auch Kondorski mit seinen Mitarbeitern stützen ihre Rechnungen auf der Theorie des polaren Metallmodells. Kaplan, der in seinen Rechnungen die von ihm erweiterte Methode von Anderson (1952) benutzt, nimmt an, dass im allgemeinen die Spin-

wellenamplituden bei den sechs Arten von Gitterplätzen im Spinell ungleich sind. Bei dieser Annahme erhielt er eine aus sechs Energiezweigen bestehende Dispersionsformel, von denen viere vom Quadrat der Wellenzahl K abhängen und zwei gleich grosse konstante Grössen sind.

Wenn man gleiche Spinwellenamplituden bei den Gitterplätzen A und gleich grosse Amplituden, wenn auch nicht dieselben, bei den Gitterplätzen B voraussetzt, da erhält man nur zwei Energiezweige.

Kaplan behauptet, dass die Annahme gleicher Amplituden in den Bewegungsgleichungen zur Formel $E \sim K^2$, und dieselbe Voraussetzung im Hamiltonian, im Falle gleich grosser Spins, zur Formel $E \sim K$ führt (siehe Kowalewski 1961). Kaplan sieht den Fehler von Wonsowski u. Seidow darin, dass Sie im Hamiltonian unrechtmässig gleich grosse Amplituden annehmen.

In der vorliegenden Arbeit wird mit Hilfe der Methode von Holstein u. Primakoff die Dispersionsformel für Spinwellen berechnet. Es wird gezeigt, dass, im Falle gleicher Spins, die Energie der Spinwellen auch bei der von Wonsowski u. Seidow eingeführten Annahme von gleichen Amplituden vom Quadrat der Wellenzahl K abhängt.

II. Der Hamiltonian und seine Eigenwerte

Die Berechnung der Erregungen nach der Theorie des polaren Metall-modells (Bogoliubow 1949) ist völlig gleichwertig der Methode von Holstein u. Primakoff (1940), wenn ausschliesslich Spinnerregungen vorliegen. Der Hamiltonian von Bogoliubow (1949, Formel 4.109) geht in diesem Falle über in die Diracsche Formel für beliebige Spins.

Der Hamiltonian hat also folgende Form:

$$\hat{H} = G_0 - \frac{1}{2} \sum_{(f_1, f_2)} J(f_1, f_2) \hat{S}_{f_1} \cdot \hat{S}_{f_2} \quad (1)$$

$J(f_1, f_2)$ Superaustauschintegral zwischen den Gitterplätzen f_1 und f_2 ;

\hat{S}_f Spinoperator beim Gitterplatz f in $\frac{\hbar}{2}$;

f Index der „magnetischen“ Gitterplätze.

Wir gehen zu den Bose-Operatoren \hat{b} über:

$$\begin{aligned} \hat{S}_f^x &= \sqrt{S_f} [g(\hat{n}_f) \hat{b}_f + \hat{b}_f^* g(n_f)] \\ \hat{S}_f^y &= i\eta_f \sqrt{S_f} [g(\hat{n}_f) \hat{b}_f - \hat{b}_f^* g(n_f)], \\ \hat{S}_f^z &= \eta_f (2\hat{b}_f^* \hat{b}_f - S_f), \end{aligned} \quad (2)$$

$$g(\hat{n}_f) = \sqrt{1 - \frac{\hat{n}_f}{S_f}}, \quad \hat{n}_f = \hat{b}_f^* \hat{b}_f, \quad S_r = \sigma, \quad S_l = S, \quad S_m = s.$$

$\eta_f = 1$ für f welches einen Oktaeder-Gitterplatz l oder m bezeichnet;

$\eta_f = -1$ für f welches einen Tetraeder-Gitterplatz r bezeichnet.

Das Spinell-Gitter ist aus sechs Translationsteilgittern zusammengesetzt. Die Vektoren der elementaren Translationen haben folgende Form (siehe Abb. 1):

$$\vec{a}_1 = \frac{a}{2} (\vec{e}_x + \vec{e}_y), \quad \vec{a}_2 = \frac{a}{2} (\vec{e}_y + \vec{e}_z), \quad \vec{a}_3 = \frac{a}{2} (\vec{e}_x + \vec{e}_z),$$

$\vec{e}_x, \vec{e}_y, \vec{e}_z$ — Einheitsvektoren,

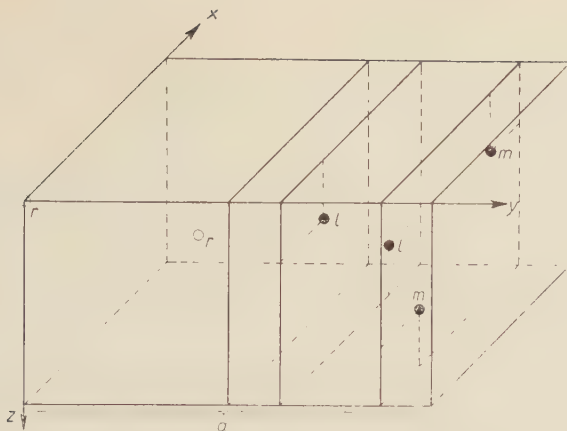


Abb. 1. Elementarzelle eines Spinells.

Lagevektoren der Tetraeder-Gitterplätze:

$$\vec{R}_r(n) = \vec{R}_n + \vec{\varrho}_r, \quad \vec{\varrho}_{r_1} = \vec{0},$$

$$\vec{R}_n = \sum_{j=1}^3 n_j \vec{a}_j, \quad \vec{\varrho}_{r_2} = \frac{a}{4} (\vec{e}_x + \vec{e}_y + \vec{e}_z),$$

$$n_j = 1, 2, \dots, N_j, \quad N_1 N_2 N_3 = \frac{N}{6},$$

N Gesamtzahl der „magnetischen“ Gitterplätze.

Lagevektoren der Oktaeder-Gitterplätze:

$$\vec{R}_l(n) = \vec{R}_n + \vec{\varrho}_l, \quad \vec{\varrho}_{l_1} = \frac{a}{8} (\vec{e}_x + 5\vec{e}_y + \vec{e}_z),$$

$$\vec{\varrho}_{l_2} = \frac{a}{8} (3\vec{e}_x + 5\vec{e}_y + 3\vec{e}_z),$$

$$\vec{R}_m(n) = \vec{R}_n + \vec{\varrho}_m, \quad \vec{\varrho}_{m_1} = \frac{a}{8} (3\vec{e}_x + 7\vec{e}_y + \vec{e}_z),$$

$$\vec{\varrho}_{m_2} = \frac{a}{8} (\vec{e}_x + 7\vec{e}_y + 3\vec{e}_z).$$

Wegen der Bedingung der Quasisättigung erhält man aus (1):

$$\begin{aligned} \hat{H} = E_0 + \sum_r [2\sigma \sum_{r'} J(r, r') - 2S \sum_l J(r, l) - 2s \sum_m J(r, m)] \hat{b}_r^* \hat{b}_r + \sum_l [2S \sum_{l'} J(l, l') - \\ - 2\sigma \sum_r J(l, r) + 2s \sum_m J(l, m)] \hat{b}_l^* \hat{b}_l - \sum_m [2s \sum_{m'} J(m, m') - 2\sigma \sum_r J(m, r) + 2S \sum_l J(m, l)] \hat{b}_m^* \hat{b}_m - \\ - 2\sigma \sum_{(r, r')} J(r, r') \hat{b}_r^* \hat{b}_{r'} - 2S \sum_{(l, l')} J(l, l') \hat{b}_l^* \hat{b}_{l'} - 2s \sum_{(m, m')} J(m, m') \hat{b}_m^* \hat{b}_{m'} \end{aligned}$$

$$\begin{aligned}
& -2\sqrt{\sigma S} \sum_{(r,l)} J(r,l) (\hat{b}_r^* \hat{b}_l^* + \hat{b}_r \hat{b}_l) - 2\sqrt{\sigma s} \sum_{(r,m)} J(r,m) (\hat{b}_r^* \hat{b}_m^* + \hat{b}_r \hat{b}_m) - \\
& -2\sqrt{sS} \sum_{(l,m)} J(l,m) \hat{b}_l^* \hat{b}_m^* - 2\sqrt{sS} \sum_{(l,m)} J(l,m) \hat{b}_m^* \hat{b}_l
\end{aligned} \quad (3)$$

wo

$$\begin{aligned}
E_0 = G_0 - \frac{1}{2} \sigma^2 \sum_{r_1 \neq r_2} J(r_1, r_2) - \frac{1}{2} S^2 \sum_{l_1 \neq l_2} J(l_1, l_2) - \frac{1}{2} s^2 \sum_{m_1 \neq m_2} J(m_1, m_2) + \sigma S \sum_{r,l} J(r, l) + \\
+ \sigma s \sum_{r,m} J(r, m) - sS \sum_{l,m} J(l, m).
\end{aligned}$$

Wenn wir im Hamiltonian (3) $J_{f_1, f_2} = \frac{1}{4} J(f_1, f_2)$ setzen, ist er bei der Voraussetzung $\sigma = S = s$ identisch mit dem Hamiltonian von Wonsowski (W.S.1.7.). Bei der Annahme $\sigma = S = s = 1$ ist er identisch mit dem Hamiltonian von Kondorski (K.10) oder (K.24).

Um den Hamiltonian (3) zu diagonalisieren, zerlegen wir die Operatoren \hat{b} in eine Fourier-Reihe.

Vektoren des inversen Gitters:

$$\begin{aligned}
\vec{K}_\lambda = \sum_{j=1}^3 \frac{2\pi\lambda_j}{N_j} \vec{a}^j, \quad -\frac{1}{2} N_j < \lambda_j \leq \frac{1}{2} N_j, \\
\vec{a}_j \cdot \vec{a}^{j'} = \delta_{jj'}.
\end{aligned}$$

Nehmen wir an, dass die Fourier-Transformaten der Operatoren \hat{b}_{r_1} und \hat{b}_{r_2} gleich gross und gleich \hat{b}_λ sind. Nehmen wir ebenso an, dass die Fourier-Transformaten der Operatoren \hat{b}_{l_1} , \hat{b}_{l_2} , \hat{b}_{m_1} , \hat{b}_{m_2} gleich gross und gleich \hat{c}_λ sind.

Die Transformationen haben dann folgende Form:

$$\begin{aligned}
\hat{b}_r &= \sqrt{\frac{3}{N}} \sum_\lambda e^{i\vec{K}_\lambda \cdot \vec{R}_r} \hat{b}_\lambda, \\
\hat{b}_l &= \sqrt{\frac{3}{2N}} \sum_\lambda e^{i\vec{K}_\lambda \cdot \vec{R}_l} \hat{c}_\lambda, \\
\hat{b}_m &= \sqrt{\frac{3}{2N}} \sum_\lambda e^{i\vec{K}_\lambda \cdot \vec{R}_m} \hat{c}_\lambda.
\end{aligned} \quad (4)$$

Die Operatoren \hat{b}_λ , \hat{c}_λ erfüllen folgende Beziehungen:

$$\hat{b}_\lambda \hat{b}_{\lambda'}^* - \hat{b}_{\lambda'}^* \hat{b}_\lambda = \hat{c}_\lambda \hat{c}_{\lambda'}^* - \hat{c}_{\lambda'}^* \hat{c}_\lambda = \delta_{\lambda\lambda'}.$$

Den Hamiltonian (3) können wir jetzt in der Form

$$\hat{H} = E_0 + \sum_\lambda A_\lambda \hat{b}_\lambda^* \hat{b}_\lambda + \sum_\lambda B_\lambda \hat{b}_\lambda \hat{c}_\lambda + \sum_\lambda B_\lambda^* \hat{b}_\lambda^* \hat{c}_\lambda^* + \sum_\lambda D_\lambda \hat{c}_\lambda^* \hat{c}_\lambda \quad (5)$$

schreiben, wo

$$\begin{aligned}
 A_\lambda &= 2\sigma \sum_{r'} J(r, r') [1 - \exp i\vec{K}_\lambda \cdot (\vec{R}_r - \vec{R}_{r'})] - 2S \sum_l J(r, l) - 2s \sum_m J(r, m), \\
 B_\lambda &= -\sqrt{\frac{\sigma}{2}} \sum_{p=1}^2 \left[\sqrt{S} \sum_l J(r_p, l) \exp i\vec{K}_\lambda \cdot (\vec{R}_{r_p} - \vec{R}_l) + \right. \\
 &\quad \left. + \sqrt{s} \sum_m J(r_p, m) \exp i\vec{K}_\lambda \cdot (\vec{R}_{r_p} - \vec{R}_m) \right], \\
 D_\lambda &= \frac{1}{2} \sum_{p=1}^2 \left\{ S \sum_l J(l_p, l) [1 - \exp i\vec{K}_\lambda \cdot (\vec{R}_l - \vec{R}_{l_p})] + \right. \\
 &\quad \left. + s \sum_m J(m_p, m) [1 - \exp i\vec{K}_\lambda \cdot (\vec{R}_m - \vec{R}_{m_p})] + S \sum_l J(m_p, l) \left[1 - \right. \right. \\
 &\quad \left. \left. - \sqrt{\frac{s}{S}} \exp i\vec{K}_\lambda \cdot (\vec{R}_l - \vec{R}_{m_p}) \right] + s \sum_m J(l_p, m) \left[1 - \sqrt{\frac{S}{s}} \exp i\vec{K}_\lambda \cdot (\vec{R}_m - \vec{R}_{l_p}) \right] \right\} - \\
 &\quad - \sigma \sum_r J(l, r) - \sigma \sum_r J(m, r)
 \end{aligned} \tag{6}$$

Wir vernachlässigen den Einfluss der Kristalloberfläche.

Den Hamiltonian (5) diagonalisieren wir mit Hilfe der Transformationen:

$$\begin{aligned}
 \hat{b}_\lambda &= \frac{1}{\sqrt{2}} (\hat{Q}_\lambda + i\hat{P}_\lambda), & \hat{c}_\lambda &= \frac{1}{\sqrt{2}} (\vec{R}_\lambda + i\vec{S}_\lambda), \\
 \hat{Q}_\lambda &= (1+w)^{-1} (w\hat{q}_{1\lambda} + \hat{q}_{2\lambda}), & \hat{P}_\lambda &= (1-w)^{-1} (-w\hat{p}_{1\lambda} + \hat{p}_{2\lambda}), \\
 \hat{R}_\lambda &= (1+w)^{-1} (\hat{q}_{1\lambda} + w\hat{q}_{2\lambda}), & \hat{S}_\lambda &= (1-w)^{-1} (\hat{p}_{1\lambda} - w\hat{p}_{2\lambda}).
 \end{aligned}$$

Den Parameter w bestimmen wir aus den Gleichungen (Tessman 1952):

$$B_\lambda w^2 + (A_\lambda + D_\lambda)w + B_\lambda = 0.$$

Wir erhalten die Eigenwerte:

$$E = \text{const} - \frac{1}{2} \sum_\lambda [A_\lambda + D_\lambda - \sqrt{(A_\lambda + D_\lambda)^2 - 4B_\lambda^2}] + \sum_\lambda E_{1\lambda} n_{1\lambda} + \sum_\lambda E_{2\lambda} n_{2\lambda} \tag{7}$$

wo

$$\begin{aligned}
 E_{1\lambda} &= \frac{1}{2} [D_\lambda - A_\lambda + \sqrt{(A_\lambda + D_\lambda)^2 - 4B_\lambda^2}], \\
 E_{2\lambda} &= \frac{1}{2} [A_\lambda - D_\lambda + \sqrt{(A_\lambda + D_\lambda)^2 - 4B_\lambda^2}], \\
 n_{1\lambda} &= 0, 1, 2, \dots, & n_{2\lambda} &= 0, 1, 2, \dots
 \end{aligned} \tag{7a}$$

Kondorski mit seinen Mitarbeitern erhielten die Größen A_k , B_k , C_k , D_k (siehe Formel K. 18).

Wenn wir die Ausdrücke (K. 18) korrigieren, indem wir die Spinellstruktur berücksichtigen, und in den Formeln (6) $\sigma = S = s = 1$ setzen, da erhalten wir folgende Beziehungen:

$$A_k = A_\lambda, \quad B_k = \sqrt{2} B_\lambda, \quad C_k = \frac{1}{\sqrt{2}} B_\lambda, \quad D_k = D_\lambda.$$

Man sieht dann leicht, dass die Dispersionsformeln von Kondorski (K. 17) mit den Formeln (7a) (für $\sigma = S = s = 1$) identisch sind.

Wenn wir in der Arbeit von Wonsowski und Seidow in den Transformationen (W. S. 1.8) die Normierungsfaktoren korrigieren, in A'_λ , B'_λ , D'_λ (W. S. 1.9) die Rechnungsfehler beseitigen, und die Superaustauschintegrale $J_{f_1 f_2}$ durch die Integrale $-\frac{1}{4} J(f_1, f_2)$ ersetzen, so wird die Dispersionsformel (W. S. 1.17) identisch mit dem Ausdruck (7), wenn $\sigma = S = s$ ist.

Man sieht also, dass die korrigierten Arbeiten von Wonsowski und Seidow und von Kondorski, Pachomow und Siklós zu denselben Resultaten führen (für Spins vom Werte 1).

Wenn wir uns beim Rechnen zu den nächsten Nachbarn und zu langen Spinwellen (kleines K) beschränken, so erhalten wir eine folgende Dispersionsformel:

$$E_{i\lambda} = \Omega_0^{(i)} + \Omega_1^{(i)} a^2 K^2 + \Omega_2^{(i)} a^2 (K^y)^2 + \Omega_3^{(i)} a^2 K^x K^z \quad (8)$$

wo

$$\begin{aligned} \Omega_0^{(2)} &= (3\alpha)^{-1} \left[18\alpha^2 J_{AB} + \frac{J_{BB}}{J_{AB}} \beta (\beta J_{BB} - 6\delta J_{AA}) \right] \pm 6J_{AB}(S + s + \sigma) \pm 2J_{BB}\beta, \\ \Omega_1^{(2)} &= \pm \frac{1}{32} (\gamma J_{BB} - 4\sigma J_{AA}) : (96\alpha)^{-1} [33\sigma(\sqrt{S} + \sqrt{s})^2 J_{AB} + (\gamma J_{BB} - 4\sigma J_{AA})(\beta - 3\delta)], \\ \Omega_2^{(2)} &= -\beta J_{BB} \left[\pm \frac{1}{32} + (96\alpha)^{-1} \left(\beta \frac{J_{BB}}{J_{AB}} - 3\delta \right) \right], \\ \Omega_3^{(2)} &= \frac{1}{16} (S - s) \left\{ \pm J_{BB} - (3\alpha)^{-1} \left[15\sigma J_{AB} + (3\delta - \beta) J_{BB} \frac{J_{BB}}{J_{AB}} \right] \right\}, \end{aligned} \quad (8a)$$

$$\alpha = \sqrt{\sigma^2 + S^2 + s^2 + 2Ss - 4\sigma\sqrt{Ss}} \neq 0,$$

$$\beta = S + s - 2\sqrt{Ss}, \quad \delta = S + s + \sigma, \quad \gamma = S + s + 2\sqrt{Ss}.$$

J_{AA} , J_{AB} , J_{BB} — Superaustauschintegrale zwischen nächsten Nachbarn $A - A$, $A - B$, $B - B$.

Die Dispersionsformel (8) mit den Koeffizienten (8a) ist anisotrop.

Die Anisotropie der Dispersionsformel (8) ist durch die magnetische Überstruktur verursacht.

Im Falle $S = s$ ($\sigma \neq 2S$) erhalten wir:

$$\Omega_0^{(1)} = 12(2S - \sigma)J_{AB},$$

$$\Omega_0^{(2)} = \Omega_2^{(1)} = \Omega_3^{(1)} = 0,$$

$$\Omega_1^{(1)} = \pm \frac{1}{8}(SJ_{BB} - \sigma J_{AA}) + \frac{1}{24}(2S - \sigma)^{-1}[33S\sigma J_{AB} - 3(2S + \sigma)(SJ_{BB} + \sigma J_{AA})] \quad (8b)$$

Die Formel (8) mit den Koeffizienten (8b) ist isotrop.

Wenn $\sigma = S = s$ ist, so erhalten wir:

$$\Omega_0^{(1)} = 12SJ_{AB},$$

$$\Omega_0^{(2)} = \Omega_2^{(1)} = \Omega_3^{(1)} = 0,$$

$$\Omega_1^{(1)} = \frac{33}{24}SJ_{AB} - \frac{1}{4}S(J_{BB} + 2J_{AA}),$$

$$\Omega_1^{(2)} = \frac{33}{24}SJ_{AB} - \frac{1}{4}S(J_{AA} + 2J_{BB}). \quad (8c)$$

In der Arbeit von Wonsowski und Seidow kann man dieselbe Abhängigkeit $E \sim k^2$ erhalten, wenn man in ihr: 1) die schon Oben erwähnten Fehler beseitigt; 2) wenn man auf richtige Weise die Kristallstruktur berücksichtigt und die Rechnungsfehler in der Näherungsberechnung der Dispersionsformel beseitigt.

Wenn $\sigma = 2S = 2s$ ist, d.h. im Falle eines Antiferromagnetikums, und wenn man nur die A—B Wechselwirkung berücksichtigt, so erhalten wir die lineare Dispersionsformel:

$$E_{1\lambda} = E_{2\lambda} = \sqrt{33}SJ_{AB} \cdot aK. \quad (9)$$

Herrn Prof. Dr S. Szczeniowski danke ich für wertvolle und nützliche Diskussionen.

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КРИТИЧЕСКИЕ МАГНИТНЫЕ ПОЛЯ ТОНКИХ СВИНЦОВЫХ ПЛЁНОК

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Были измерены критические магнитные поля для тонких плёнок свинца в температурном интервале, равном около 1,2 К ниже критической температуры свинца. Измерялись плёнки толщиной $3,15 \cdot 10^{-6}$ см — $1,16 \cdot 10^{-4}$ см. Для тонких плёнок фазовые переходы из сверхпроводящего состояния в нормальное или наоборот, в присутствии магнитного поля — обратимы. Для толстых плёнок переходы обратимы лишь вблизи критической температуры T_K , тогда как для температур, более отдалённых от T_K , переходы сопровождаются появлением гистерезиса. Уже при температурах близких T_K получено максимальное значение гистерезиса.

§ 1 Введение

Свойства сверхпроводников, которые по размерам сравнимы с глубиной проникновения магнитного поля в массивный сверхпроводник ($\delta \sim 10^{-6}$ см), отличаются от свойств массивных сверхпроводников.

Впервые исследования тонких плёнок сверхпроводников были проведены независимо А. И. Шальниковым [1] [2] и Эпплярдом, Бристоу, Г. Лондоном и Мизером [3] [4] [5].

Шальников, в результате исследований тонких плёнок олова, свинца и таллия толщиной $5 \cdot 10^{-7}$ см — $3 \cdot 10^{-5}$ см, пришёл к выводу, что величины критических полей для тонких плёнок значительно больше, чем для случая массивного металла. Измерения для свинца проводились лишь при температурах ниже 4,2° К.

Проводя подобные исследования для тонких плёнок ртути, Эпплярд, и соавторы нашли значительное увеличение критических магнитных полей по сравнению с массивным металлом; кроме этого, в своей работе они приводят зависимость отношения критического магнитного поля тонкой плёнки H_K к критическому магнитному полю массивного металла H_{KM} от толщины плёнки d .

Эта зависимость имеет следующий вид:

$$\frac{H_K}{H_{KM}} = 1 + \frac{b}{d} \quad (1)$$

(553)

b — равно приблизительно $1,2 \cdot 10^{-5}$ см при низких температурах и зависит от температуры так же, как глубина проникновения магнитного поля.

Зависимость (1), подтверждённая также с помощью опытов Эндрю [6] и Локка [7], справедлива лишь для толстых плёнок, причём величина b не сохраняется при изменении сверхпроводника.

Неудачной оказалась попытка Гинзбурга [8] найти также зависимость $\frac{H_K}{H_{KM}}$ для более тонких плёнок, пользуясь феноменологической теорией сверхпроводимости Ф. Лондона и Г. Лондона [9].

Гинзбургом и Ландау [10] была разработана другая форма макроскопической теории сверхпроводимости, в которой, кроме свойств массивных сверхпроводников, была разработана проблема сверхпроводимости образцов малых размеров.

Из теории Гинзбурга-Ландау следуют особенные свойства тонких сверхпроводящих плёнок, находящихся в магнитном поле.

Согласно этой теории, плёнки, в зависимости от толщины, можно разделить на два класса: $d < d_K$ и $d > d_K$, где d_K является некоторой критической толщиной.

Для тонких плёнок ($d < d_K$) переход из сверхпроводящего состояния в нормальное или наоборот, в присутствии магнитного поля, является фазовым переходом второго рода. Для тонких плёнок справедлива следующая зависимость:

$$\frac{H_K}{H_{KM}} = 2\sqrt{6} \frac{\delta}{d} \quad (2)$$

Для случая толстых плёнок ($d > d_K$) переход из сверхпроводящего состояния в нормальное или обратно является фазовым переходом первого рода, причём для плёнок с $d \gg d_K$ выполняется зависимость:

$$\frac{H_K}{H_{KM}} = 1 + \frac{\delta}{d} \quad (3)$$

Заварицкий, проводя измерения на тонких плёнках олова [11], таллия и индия [12], полностью подтвердил выводы, следующие из теории Гинзбурга-Ландау.

В настоящей работе приводятся результаты измерений магнитных критических полей для случая тонких плёнок свинца.

§ 2. Экспериментальная часть

С целью получения температур выше 4,2° К, был построен криостат, представленный на рис. 1. Похожий криостат был предложен Заварицким [13]. Применение автоматического фотоэлектрического усилителя для питания нагревателя позволяло поддерживать температуру с точностью 0,0005° К в течение довольно долгого промежутка времени.

Для измерения температуры был использован угольный термометр сопротивления, сделанный из радиотехнического сопротивления типа Аллена-Брэдли.

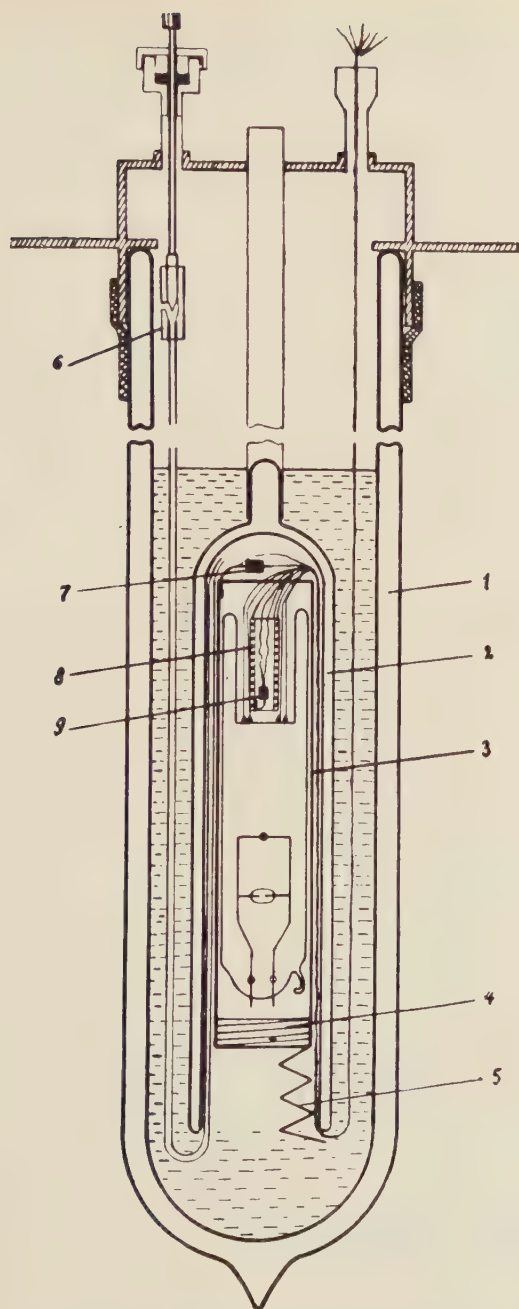


Рис. 1. Криостат для температур выше $4,2^{\circ}\text{K}$

1 — сосуд Дюара с жидким гелием, 2 — перевернутый дюаровский сосуд, 3 — Экран из медной фольги, 4 — нагреватель, 5 — медная полоска, соединяющая экран с жидким гелием, 6 — вентиль, 7 и 9 — угольные термометры, 8 — катушка из свинцовой проволоки. На рисунке нет внешнего дюаровского сосуда с жидким азотом.

Сопротивление использовавшегося термометра, изменявшееся в температурном интервале 6,2 К—7,2 К на 9900 омов, измерялось с помощью высокоомного потенциометра. Градуировочная кривая термометра контролировалась перед каждым экспериментом в двух точках: температуре кипения жидкого гелия под атмосферным давлением и точке перехода массивного свинца из сверхпроводящего в нормальное состояние (7,22°К). Для исследований употреблялся свинец высокой чистоты, не меньше, чем 99,999%, что было проверено спектральными и химическими методами.

Образцы были получены путём конденсации свинца в вакууме на плоских, оптически полированных стеклянных подложках. Четыре платиновых провода, пропаянные сквозь подложки, использовались в качестве токовых и потенциальных проводов для измерения сопротивления плёнок.

Толщина плёнок определялась весом испарённого металла.

Для определения перехода образцов из сверхпроводящего в нормальное состояние измерялось изменение сопротивления образца в зависимости от температуры (рис. 2), или величины внешнего магнитного поля.

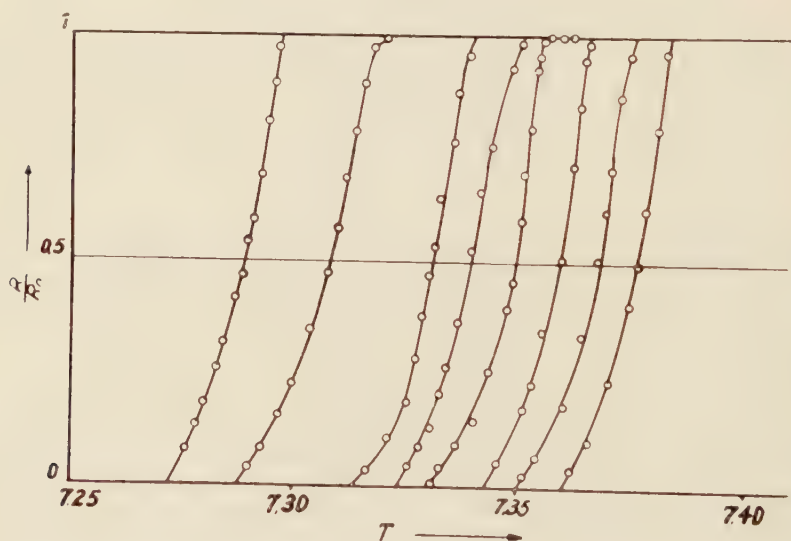


Рис. 2. Изменение сопротивления образцов разных толщин в зависимости от температуры

- R — значение сопротивления образца
 R_n — значение сопротивления образца в нормальном состоянии
 T — температура в °К.

В первом случае определялась температура перехода T_K плёнки, во втором — значение критического магнитного поля H_K при определённой постоянной температуре T . В качестве T_K и H_K принимались значения, которым на определённых кривых перехода соответствовало сопротивление, равное половине сопротивления

образца в нормальном состоянии (вблизи температуры перехода). Сопротивление образцов измерялось с помощью низкоомного потенциометра.

Магнитное поле получалось с помощью катушек Гельмгольца ($H \gg 250$ эрст), или электромагнита.

Магнитное поле было установлено всегда параллельно плоскости образца.

§ 3 Результаты

Было исследовано поведение в магнитном поле шестнадцати тонких свинцовых плёнок толщиной $3,15 \cdot 10^{-6}$ см — $1,16 \cdot 10^{-4}$ см. Исследования проводились в температурном интервале $\Delta T = T_K - T$, равном для некоторых образцов около $1,2^\circ\text{K}$ (T_K — температура перехода плёнки в отсутствие магнитного поля, T — температура измерения).

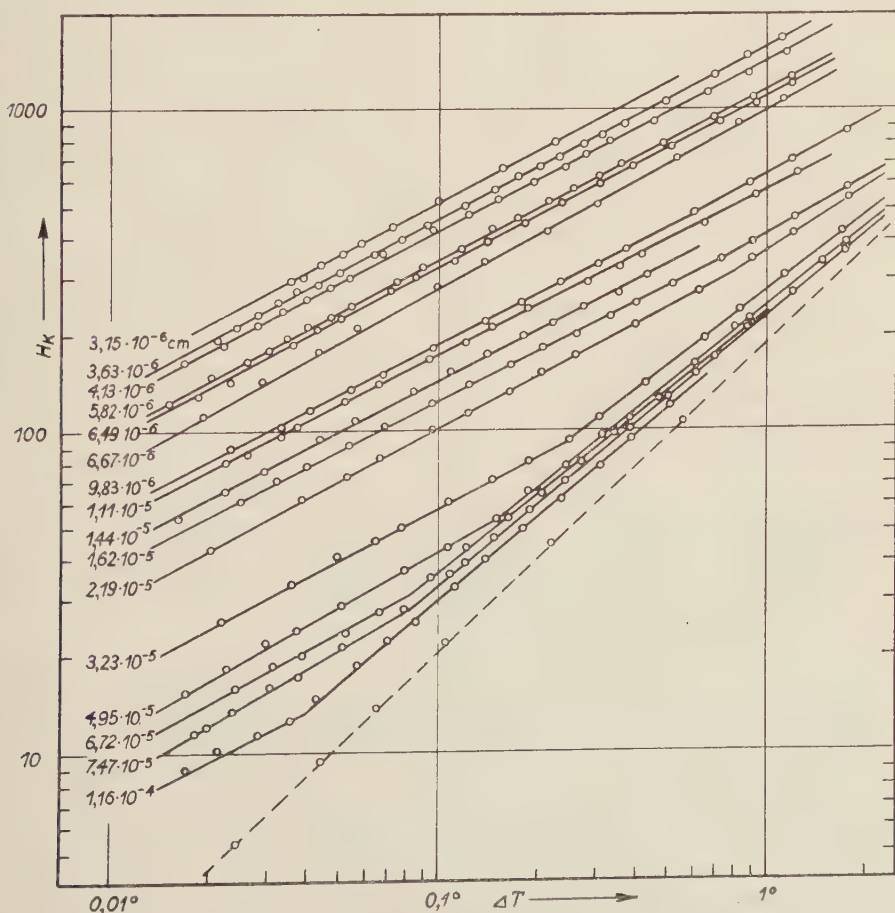


Рис. 3. Зависимость критических полей H_K от температуры ΔT . Пунктирная линия — значения критических полей H_{KM} для массивного свинца.

Температурный интервал, в котором сопротивление образцов менялось от значения R_n (в нормальном состоянии) до нуля (в сверхпроводящем состоянии), у большинства плёнок не превышал $0,03^\circ\text{K}$.

На рис. 3 показана зависимость критических магнитных полей плёнок H_K от температуры ΔT . Как видно из рис. 3, для плёнок толщиной меньше, чем $1,62 \cdot 10^{-5}$ см, сохраняется характер зависимости $H_K = f(\Delta T)$ во всём температурном интервале, причём критическое магнитное поле пропорционально $\Delta T^{1/2}$.

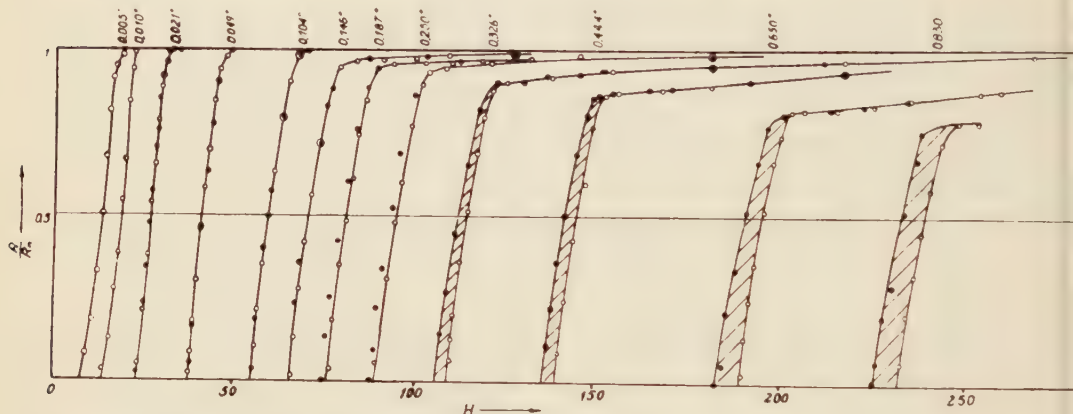


Рис. 4. Кривые перехода из сверхпроводящего в нормальное состояние в магнитном поле для плёнки толщиной $3,23 \cdot 10^{-5}$ см

H — напряжение магнитного поля в эрстедах

Цифры над кривыми перехода обозначают величины $\Delta T = T_K - T$

○ — результаты полученные при увеличении поля

● — результаты полученные при понижании поля

Область зачерченная — область гистерезиса.

Для плёнок толщиной больше чем $1,62 \cdot 10^{-5}$ см на кривых зависимости $H_K = f(\Delta T)$ наблюдается излом; влево от излома характер зависимости $H_K = f(\Delta T)$ сохраняется таким же, как и у плёнок тоньше чем $1,62 \cdot 10^{-5}$ см; напротив, вправо от излома зависимость $H_K = f(\Delta T)$ похожа на зависимость, характерную для массивного металла (пунктирная линия на рис. 3).

Было найдено, что для плёнок тоньше $1,62 \cdot 10^{-5}$ см фазовые переходы из сверхпроводящего состояния в нормальное, происходящие в присутствии магнитного поля, — обратимы. Наоборот, для плёнок более толстых, чем $1,62 \cdot 10^{-5}$ см, фазовые переходы обратимы только вблизи критической температуры плёнки; начиная с определённого значения ΔT , наблюдается явление гистерезиса: значения магнитных критических полей при переходах из сверхпроводящего состояния в нормальное больше, чем значения при обратных переходах (рис. 4 и 5). Как видно из рис. 4, область гистерезиса увеличивается с ростом ΔT , стремясь к постоянному значению. В таком поведении состоит разница между свинцом с одной стороны и оловом [11] и индием [12] с другой.

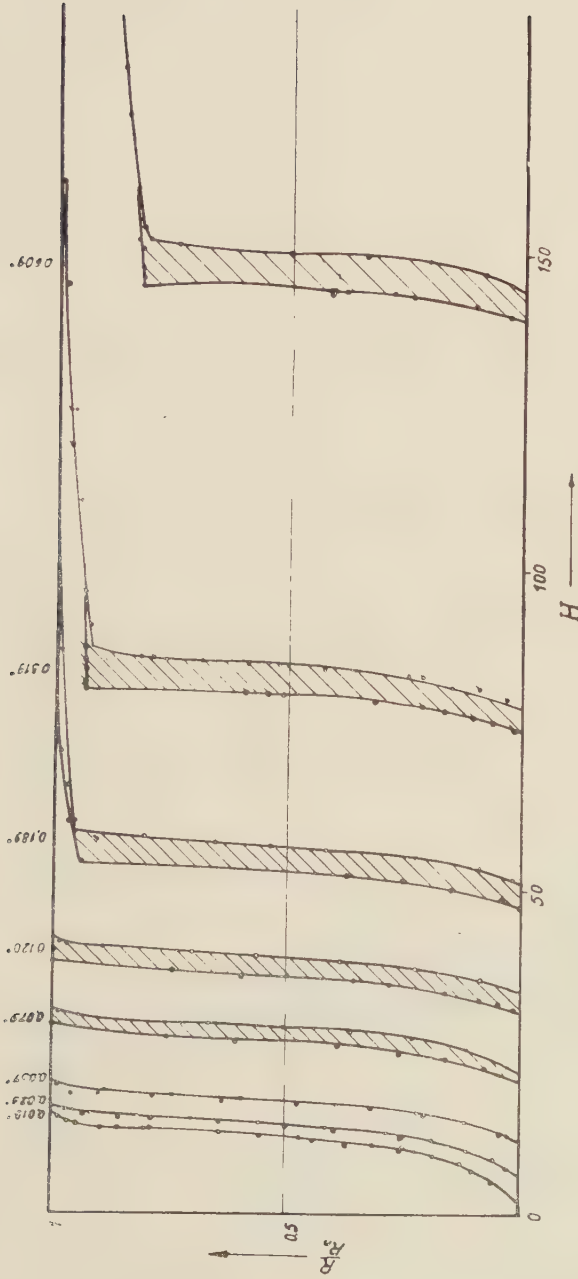


Рис. 5. Кривые перехода для плёнки толщиной $7,47 \cdot 10^{-5}$ см

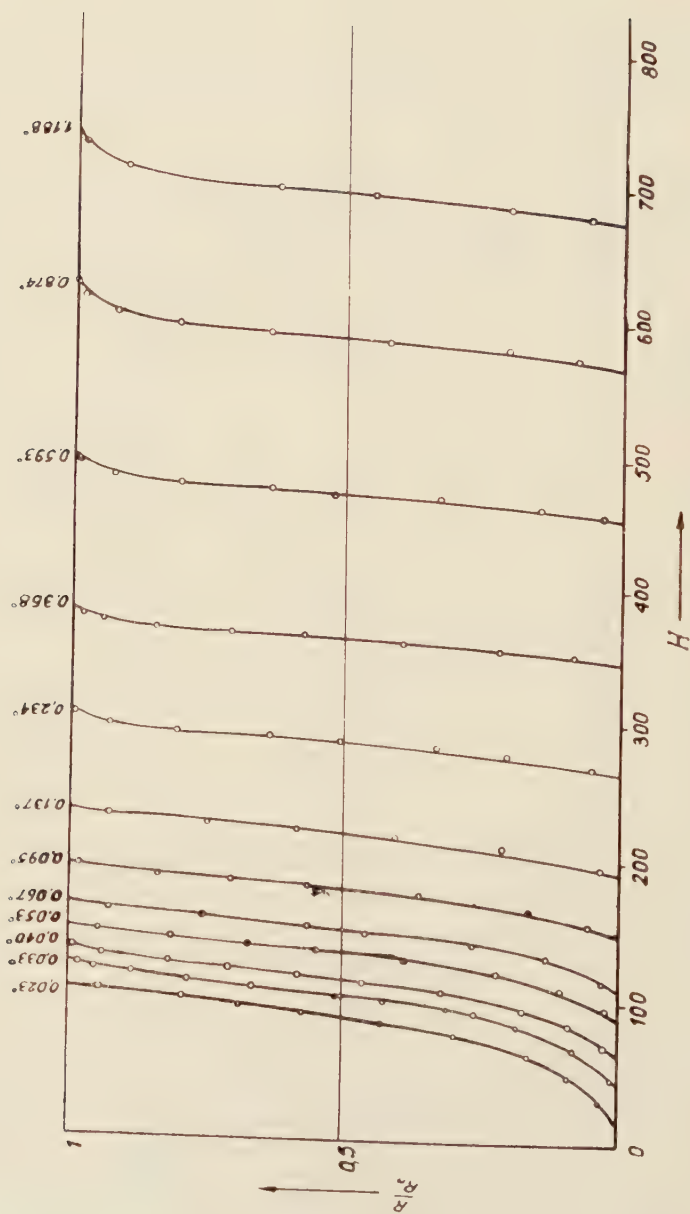


Рис. 6. Кривые перехода для плёнки толщиной $9.83 \cdot 10^{-6}$ см

Было замечено, что для тонких плёнок переходы из сверхпроводящего в нормальное состояние и наоборот являются крутыми (рис. 6). Для более толстых плёнок крутые переходы характерны лишь вблизи критической температуры; начиная с определённой температуры T_c , сопротивление растёт круто от нуля до некоторого значения меньшего, чем значение сопротивления образца в нормальном состоянии. При дальнейшем увеличении магнитного поля сопротивление очень медленно растёт, вплоть до величины сопротивления R_n , а затем не претерпевает последующих изменений.

Такое поведение более толстых плёнок может быть связано, как нам кажется, с возможностью возникновения промежуточного состояния для свинцовых плёнок. Более определенно этот вопрос могут решить дальнейшие исследования.

Автор выражает глубокую благодарность А. И. Шальникову за постоянную помощь во время выполнения этой работы в криогенной лаборатории Московского Государственного Университета.

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ТЕМПЕРАТУРНАЯ ЗАВИСИМОСТЬ ГЛУБИНЫ ПРОНИКНОВЕНИЯ МАГНИТНОГО ПОЛЯ В СВЕРХПРОВОДЯЩИЙ СВИНЕЦ

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На основании измерений критических магнитных полей тонких плёнок свинца приводится температурная зависимость глубины проникновения магнитного поля в сверхпроводящий свинец. Экстраполируя полученные значения к $T=0^\circ\text{K}$, автор получил значение $\delta_0 = (4,5 \pm 0,2) \cdot 10^{-6}$ см.

До сих пор в литературе встречается мало работ, посвящённых измерению глубины проникновения магнитного поля в сверхпроводящий свинец.

На основании опытов по измерению сопротивления тонких свинцовых проволок Понтиус [1] определил величину глубины проникновения магнитного поля с точностью до порядка $(10^{-5} - 10^{-6})$ см.

Стиль [2], исследуя магнитную проницаемость сверхпроводящих свинцовых шариков радиусом порядка 10^{-3} см и используя зависимости, вытекающие из теории Ф. Лондона и Г. Лондона [3], определил величину глубины проникновения магнитного поля при температуре $4,22^\circ\text{K}$. Согласно его данным она равна $(1,3 \pm 0,3) \cdot 10^{-5}$ см.

Локк [4], используя теорию Ф. Лондона и Г. Лондона для полученных им экспериментально магнитных моментов тонких плёнок при температуре $4,24^\circ\text{K}$, вычислил глубины проникновения для пяти свинцовых образцов.

Принимая температурную зависимость глубины проникновения магнитного поля, которая следует из теории Гортера и Казимира [5].

$$\delta = \frac{\delta_0}{\sqrt{1 - \left(\frac{T}{T_K}\right)^4}} \quad (1)$$

где δ_0 — значение глубины проникновения при $T = 0^\circ\text{K}$

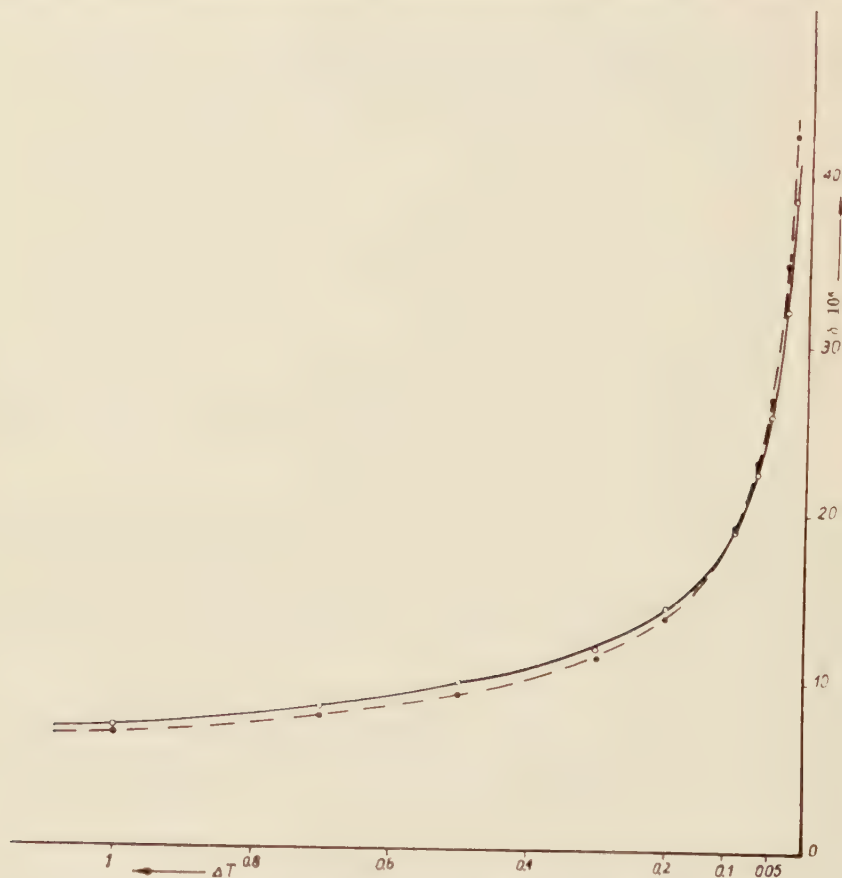
T — температура

T_K — критическая температура

последний получил для δ_0 величину, равную $(3,9 \pm 0,3) \cdot 10^{-6}$ см.

Симон [6], используя результаты измерений поверхностного импеданса на частоте 9200 мГц и формулы из теории Ф. Лондона и Г. Лондона, представил графически температурные зависимости глубины проникновения.

Глубины проникновения магнитного поля, полученные из измерений активного и реактивного сопротивления, отличаются между собой во всём температур-



Температурная зависимость глубины проникновения магнитного поля для свинца. Непрерывная линия — результаты автора Пунктирная линия — построена по формуле (1)

ном интервале. Экстраполяция значения глубины проникновения для $T = 0^\circ\text{K}$ даёт значение $\delta_0 = 5,4 \cdot 10^{-6}\text{см}$.

На основании измерений магнитных критических полей тонких плёнок свинца, выполненных автором [7], также можно вычислить и дать графическое представление её изменения с температурой. Для этой цели удобно использовать зависимость:

$$\frac{H_K}{H_{KM}} = 2\sqrt{6} \frac{\delta}{d} \quad (2)$$

вытекающую из теории Гинзбурга и Ландау [8],

где: H_K — критическое магнитное поле тонкой плёнки
 H_{KM} — критическое магнитное поле массивного металла
 δ — глубина проникновения магнитного поля
 d — толщина плёнки

Необходимо добавить, что зависимость (2) справедлива лишь для таких тонких плёнок, для которых фазовые переходы из сверхпроводящего в нормальное состояние и наоборот являются переходами второго рода.

С помощью непрерывной линии на рисунке представлена температурная зависимость $\delta(T)$, полученная автором ($1T = T_K - T$). Пунктирная линия представляет зависимость $\delta(T)$, вычислённую из формулы (1). Экстраполируя полученные результаты измерений для δ к температуре $T = 0^\circ\text{K}$ с помощью зависимости (1), автор определил глубину проникновения магнитного поля в сверхпроводящий свинец. Полученная величина равна:

$$\delta_0 = (4,5 \pm 0,2) \cdot 10^{-6} \text{ см.}$$

и находится между значениями, полученными Локком и Симоном.

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THE CRITICAL PROBLEMS FOR MULTILAYER SLAB SYSTEMS

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In the work the solution of the critical problems for slab multilayers systems are given by the procedure developed by K. M. Case for one-velocity Boltzmann equation with isotropic scattering of neutrons. In all considered cases the solution of Boltzmann equation is reduced to the solution of one dimensional Fredholm type integral equation with an additional critical condition.

Introduction

In the report the critical problems for slab multilayer systems are solved by the procedure derived by K. M. Case [1]. The following types of problems are considered: a) multiplying slab with infinite reflector, b) three-zone core with infinite reflector and c) slab with finite reflector. In all cases symmetry with respect to the central slab is assumed. In all cases the solution of the Boltzmann equation is reduced to the solution of the Fredholm integral equation with an additional critical condition. The solution of the Fredholm equation cannot be expressed in an analytical form, an approximate method using the spherical harmonics treatment of the kernel is proposed.

1. The solution of the Boltzmann equation and the properties of eigenfunctions

One velocity Boltzmann equation in plane geometry in the case of isotropic scattering has the form

$$\mu \frac{\partial \Psi_i(x, \mu)}{\partial x} + \frac{1}{l_i} \Psi_i(x, \mu) = \frac{c_i}{2l_i} \int_{-1}^1 \Psi_i(x, \mu') d\mu' \quad (1.1)$$

where index i denotes respective region, μ is the cosine of the angle between neutron velocity and x -axis, l_i is the neutron mean free path and c_i is the number of secondaries per collision.

Following K. M. Case's [1] results we can express the solution of Eq. (1.1) in the form

$$\Psi_i(x, \mu) = a_i e^{-\frac{x}{l_i \mu}} \Phi_i(\mu, v_i) + b_i e^{\frac{x}{l_i \mu}} \Phi_i(\mu, -v_i) + \int_{-1}^1 A_i(v) e^{-\frac{x}{l_i v}} \Phi_i(\mu, v) dv \quad (1.2)$$

where

$$\Phi_i(\mu, v) = \frac{c_i}{2} \frac{v}{v - \mu} + \lambda_i(\mu) \delta(\mu - v) \quad (1.3)$$

In the later considerations all integrals involving terms of the type $\frac{1}{v - \mu}$ will be understood in the sense of the principal value. The function $\lambda_i(\mu)$ is given by the formula

$$\lambda_i(\mu) = 1 - c_i v \tan h^{-1} v \quad (1.4)$$

and $\pm v_i$ are the roots of a transcendental equation

$$c_i v_i \tan h^{-1} \frac{1}{v_i} = 1 \quad (1.5)$$

It is well known that for all c_i v_i not belonging to $(-1, 1)$ and $\Phi_i(\mu, \pm v_i)$ reduces to the form

$$\Phi_i(\mu, \pm v_i) = \frac{c_i}{2} \frac{v_i}{v_i \mp \mu} \quad (1.6)$$

The functions $A_i(v)$ and the constants a_i and b_i can be evaluated by means of the boundary conditions depending on the problem considered.

As it has been proved by K. M. Case the functions of the form (1.2) are complete in the space of solutions Eq. (1.1).

It is easily seen that the functions $\Phi_i(\mu, v)$ satisfy the following "orthogonality" relations

$$\int_{-1}^1 \mu \Phi_i(\mu, v) \Phi_k(\mu, \eta) d\mu = \eta \lambda_i(v) \lambda_k(\eta) \delta(v - \eta) + \frac{c_i - c_k}{2} \frac{v\eta}{v - \eta} \quad (1.7)$$

$$\int_{-1}^1 \mu \Phi_i(\mu, \pm v_i) \Phi_k(\mu, v) d\mu = \frac{c_i - c_k}{c_i} v \Phi_i(v, \pm v_i) \quad (1.8)$$

$$\int_{-1}^1 \mu \Phi_i(\mu, \pm v_i) \Phi_k(\mu, \pm v_k) d\mu = \begin{cases} \pm \frac{c_i - c_k}{2} \frac{v_i v_k}{v_i - v_k} & \text{for } i \neq k \\ \pm \frac{c_i}{2} (v_i)^3 \left[\frac{c_i}{(v_i)^2 - 1} - (v_i)^{-2} \right] = N_i(\pm v_i) & \text{for } i = k \end{cases} \quad (1.9)$$

and

$$\int_{-1}^1 \mu \Phi_i(\mu, \pm v_i) \Phi_k(\mu, \mp v_k) d\mu = \pm \frac{c_k - c_i}{2} \frac{v_i v_k}{v_i + v_k} \quad (1.10)$$

Putting $i = k$ we obtain the orthogonality relation derived by K. M. Case for the function defined in the same region.

Using Eqs. ((1.7)-(1.10)) and the Poincare-Bertrand theorem we obtain the following formulas necessary for further analysis

$$\int_{-1}^1 \mu \Phi_i(\mu, \pm v_i) d\mu \int_{-1}^1 Q(\eta) \Phi_k(\mu, \eta) d\eta = \frac{c_i - c_k}{c_i} \int_{-1}^1 \eta Q(\eta) \Phi_i(\eta, \pm v_i) d\eta \quad (1.11)$$

and

$$\begin{aligned} \int_{-1}^1 \mu \Phi_i(\mu, v) d\mu \int_{-1}^1 Q(\eta) \Phi_k(\mu, \eta) d\eta = v \left[\lambda_i(v) \lambda_k(v) - \frac{\pi^2}{4} c_i c_k v^2 \right] Q(v) + \\ + \frac{c_k - c_i}{2} v \int_{-1}^1 \frac{\eta Q(\eta) d\eta}{\eta - v} = v N_{ik}(v) Q(v) + \frac{c_k - c_i}{2} v \int_{-1}^1 \frac{\eta Q(\eta)}{\eta - v} d\eta \end{aligned} \quad (1.12)$$

The formulas (1.11) and (1.12) are valid for arbitrary functions $Q(v)$ which satisfy the Hölder conditions.

2. The critical problem of a slab with an infinite reflector

Let us consider an infinite slab of multiplying medium ($c > 1$) of the thickness 2ϱ with a reflector of infinite thickness on both sides of the slab. The Cartesian coordinate system with the origin in the centre plane of the slab and x -axis perpendicular to this plane is chosen.

The solutions of the Boltzmann equations will be denoted as follows: for the slab $\Psi_1(x, \mu)$ and for the reflector $\Psi_2(x, \mu)$ for $x > \varrho$ and $\Psi_3(x, \mu)$ for $x < -\varrho$. The boundary conditions in our case are as follows:

a) The solution must be continuous at the boundary between the slab and the reflector

$$\begin{aligned} \Psi_1(\varrho, \mu) &= \Psi_2(\varrho, \mu) \\ \Psi_1(-\varrho, \mu) &= \Psi_3(-\varrho, \mu) \end{aligned} \quad (2.1)$$

b) The solutions in the reflector must vanish at infinity

$$\lim_{x \rightarrow \infty} \Psi_2(x, \mu) = \lim_{x \rightarrow -\infty} \Psi_3(x, \mu) = 0 \quad (2.2)$$

The Boltzmann equation in plane geometry Eq. (1.1) is invariant with respect to the transformation of (x, μ) into $(-x, -\mu)$. The symmetry of our problem implies that the boundary conditions are also invariant with respect to this transformation. Therefore the solutions are also invariant i.e.

$$\Psi_1(x, -\mu) = \Psi_1(-x, -\mu) \quad (2.3)$$

and

$$\Psi_2(x, \mu) = \Psi_3(-x, -\mu) \quad (2.4)$$

From the above conditions we can conclude that it is sufficient to consider only the region $x > 0$. The extension to the region $x < 0$ is straightforward. Using the above results the boundary conditions can be expressed in the ultimate form

$$\Psi_1(0, \mu) = \Psi_1(0, -\mu) \quad (2.5)$$

$$\Psi_1(\varrho, \mu) = \Psi_2(\varrho, \mu) \quad (2.6)$$

and

$$\lim_{x \rightarrow \infty} \Psi_2(x, \mu) = 0 \quad (2.7)$$

From the conditions (2.5)-(2.7) the coefficients of the eigenfunction expansion can be evaluated. Inserting the function $\Psi_2(x, \mu)$ given by Eq. (1.2) into the condition (2.7) we obtain that

$$A_2(v) = 0 \quad \text{for} \quad v < 0 \quad (2.8)$$

and

$$b_2 = 0 \quad (2.9)$$

Multiplying both sides of Eq. (2.5) by $\mu\Phi_1(\mu, v)$ and $\mu\Phi_1(\mu, \pm v_1)$ respectively, and integrating with respect to μ over the interval $(-1, 1)$ we have the following relations:

$$\int_{-1}^1 \mu\Phi_1(\mu, v)\Psi_1(0, \mu)d\mu = \int_{-1}^1 \mu\Phi_1(\mu, v)\Psi_1(0, -\mu)d\mu \quad (2.10)$$

and

$$\int_{-1}^1 \mu\Phi_1(\mu, \pm v_1)\Psi_1(0, \mu)d\mu = \int_{-1}^1 \mu\Phi_1(\mu, \pm v_1)\Psi_1(0, -\mu)d\mu \quad (2.11)$$

As the functions $\Phi_1(\mu, v)$ and $\Phi_1(\mu, \pm v_1)$ are complete in the interval $(-1, 1)$ the relations (2.10) and (2.11) are equivalent to Eq. (2.5).

Using the orthogonality properties of the functions $\Phi_1(\mu, v)$ and $\Phi_1(\mu, \pm v_1)$ we obtain from (2.10) and (2.11) the following relations:

$$A_1(v) = A_1(-v) \quad (2.12)$$

and

$$a_1 = b_1 \quad (2.13)$$

Further relations can be deduced by multiplying Eq. (2.6) by the functions $\mu\Phi_2(\mu, v)$ and $\mu\Phi_2(\mu, \pm v_1)$, respectively, and integrating over $\mu \in (-1, 1)$:

$$vN_{22}(v)e^{-\frac{\rho}{lv}}A_2(v) = \int_{-1}^1 \mu\Phi_2(\mu, v)\Psi_1(\rho, \mu)d\mu \quad (2.14)$$

$$N_2(v_2)e^{-\frac{\rho}{lv_2}}a_2 = \int_{-1}^1 \mu\Phi_2(\mu, v_1)\Psi_1(\rho, \mu)d\mu \quad (2.15)$$

$$N_2(-v_2)b_2e^{+\frac{\rho}{lv_2}} = \int_{-1}^1 \mu\Phi_2(\mu, -v_1)\Psi_1(\rho, \mu)d\mu \quad (2.16)$$

$N_{22}(v)$ and $N_2(\pm v_2)$ are defined by Eqs. (1.12) and (1.9).

Eq. (2.14) for $v=0$ and Eq. (2.15) determine the coefficients of the eigenfunction expansion in the reflector region by means of the solution in the multiplying region. Eq.

(2.14) for $v < 0$ and Eq. (2.16) using Eqs. (2.8) and (2.9) can be written in the form

$$\int_{-1}^1 \mu \Phi_2(\mu, -v) \Psi_1(\varrho, \mu) d\mu = 0 \quad \text{for } v > 0 \quad (2.17)$$

and

$$\int_{-1}^1 \mu \Phi_2(\mu, -v_2) \Psi_1(\varrho, \mu) d\mu = 0 \quad (2.18)$$

These equations with the conditions (2.12) and (2.13) can be reduced to the integral equation for the function $A_1(v)$ defined in the interval (0.1) and to the additional condition. The constant a_1 cannot be evaluated in the problem considered as the system of Eqs. (2.17), (2.12), (2.13) and (2.18) is homogeneous with respect to $A_1(v)$, a_1 and b_1 . Thus all the considered equations can be divided by the constant a_1 . Ultimately the integral equation has the form

$$N_{12}(\mu) Y(\mu) + \frac{c_1 - c_2}{2} \int_0^1 \left\{ \frac{v}{v - \mu} + \frac{v e^{-\frac{2\varrho}{lv}}}{v + \mu} \right\} Y(v) dv \\ - \frac{c_1 - c_2}{c_1} \left\{ \Phi_1(\mu_1 - v_1) e^{-\frac{\varrho}{lv_1}} + \Phi_1(\mu, v_1) e^{\frac{\varrho}{lv_1}} \right\} \quad (2.19)$$

where a new unknown function given by the expression

$$Y(\mu) = \frac{A_1(v) e^{\frac{\varrho}{lv}}}{a_1} \quad (2.20)$$

is introduced.

The additional condition

$$\int_0^1 \left\{ \frac{v}{v_2 - v} + \frac{v e^{-\frac{2\varrho_1}{lv_1}}}{v_2 + v} \right\} Y(v) dv = -v_1 \left\{ \frac{e^{-\frac{\varrho}{lv_1}}}{v_1 + v_2} + \frac{e^{\frac{\varrho}{lv_1}}}{v_1 - v_2} \right\} \quad (2.21)$$

is to be considered as a critical condition. The solution of the Boltzmann equation for the reflected slab has been reduced to the solution of Eq. (2.19) with the critical condition (2.21). These equations give the angular distribution of neutrons in the multiplying medium as proportional to an arbitrary constant. The angular distribution is directly obtained by means of the above relation.

Let us consider the limiting case when $c_2 \rightarrow 0$. From the definitions we have

$$\begin{aligned} \text{a) } \lim_{c_2 \rightarrow 0} \lambda_2(v) &= 1 \\ \text{b) } \lim_{c_2 \rightarrow 0} v_2 &= \infty \\ \text{c) } \lim_{c_2 \rightarrow 0} N_{12}(v) &= \lambda_1(v) \end{aligned} \quad (2.22)$$

Putting these values into Eq. (2.19) we obtain the integral equation of the form

$$\begin{aligned} \lambda_1(\mu) Y_1(\mu) + \frac{c_1}{2} \int_0^1 \left\{ \frac{v}{v-\mu} + \frac{ve^{-\frac{2e_1}{lv}}}{v+\mu} \right\} Y(v) dv \\ = - \left\{ \Phi_1(\mu, -v_1) e^{-\frac{e}{lv_1}} + \Phi_2(\mu, v_1) e^{\frac{e}{lv_1}} \right\} \end{aligned} \quad (2.23)$$

The critical condition (2.21) tends to the identity $0=0$.

The equation (2.23) is identical with the equation derived by R. Želazny [2] in the case of a bare slab.

The equation (2.19) is a singular integral equation which can be reduced to the Fredholm equation by the method given by N.I. Muskhelishvili [3]. This Fredholm equation has a form (see App. A)

$$\begin{aligned} Y(\mu) - \frac{c_1 - c_2}{2T(\mu)} \int_0^1 ve^{-\frac{2e}{lv}} Y(v) \left\{ \frac{c_1 - c_2}{2} \int_0^1 \frac{\eta W(\eta) d\eta}{(\eta - \mu)(\eta + v)} - \frac{S(\mu)T(\mu)}{v + \mu} \right\} dv \\ = S(\mu)\Phi_d(\mu) - \frac{c_1 - c_2}{2T(\mu)} \int_0^1 \frac{\eta \Phi_d(\eta) W(\eta)}{\eta - \mu} d\eta \end{aligned} \quad (2.24)$$

where

$$S(\mu) = \frac{\lambda_1(\mu)\lambda_2(\mu) + \frac{\pi^2}{4} c_1 c_2 \mu^2}{\left[\lambda_1(\mu)\lambda_2(\mu) + \frac{\pi^2}{4} c_1 c_2 \mu^2 \right]^2 + \left[\frac{c_1 - c_2}{2} \pi \mu \right]^2} \quad (2.25)$$

$$T(\mu) = X_{12}^-(\mu) \left\{ \lambda_1(\mu)\lambda_2(\mu) + \frac{\pi^2}{4} c_1 c_2 \mu^2 + \frac{c_1 - c_2}{2} \pi i \mu \right\} \quad (2.26)$$

$$W(\mu) = X_{12}^-(\mu) \left\{ \lambda_1(\mu)\lambda_2(\mu) + \frac{\pi^2}{4} c_1 c_2 \mu^2 - \frac{c_1 - c_2}{2} \pi i \mu \right\}^{-1} \quad (2.27)$$

and

$$\Phi_d(\mu) = - \frac{c_1 - c_2}{c_1} \left\{ \Phi_1(\mu, v_1) e^{\frac{e}{lv_1}} + \Phi_1(\mu, -v_1) e^{-\frac{e}{lv_1}} \right\} \quad (2.28)$$

The function $X_{12}^-(\mu)$ is defined by Eq. (A. 9). As the index of the singular integral equation (2.19) $\kappa=0$, the equations (2.19) and (2.24) are equivalent without any additional condition.

The solution of the Fredholm equation (2.24) is not known in an analytical form. One of the possible approximate methods of solving this equation based on the spherical harmonics representation is given in App. B.

3. The critical problem of a three-zone core with an infinite reflector

Let us consider a system consisting of a central slab of the thickness $2\varrho_1$, characterized by material parameters c_1, l_1 surrounded by two symmetrical slabs of the thickness $\varrho_2 - \varrho_1$ described by material parameters c_2, l_2 . The whole system is immersed in an infinite reflector, the values of material parameters of which are denoted by c_3 and l_3 .

The origin of x -axis in the Cartesian coordinate system lies in the plane of symmetry of the system.

After a similar discussion as that of the Chapter II, the boundary conditions can be expressed in the form:

$$\Psi_1(0, \mu) = \Psi_1(0, -\mu) \quad (3.1)$$

$$\Psi_1(\varrho_1, \mu) = \Psi_2(\varrho_1, \mu) \quad (3.2)$$

$$\Psi_2(\varrho_2, \mu) = \Psi_3(\varrho_2, \mu) \quad (3.3)$$

$$\lim_{x \rightarrow \infty} \Psi_3(x, \mu) = 0 \quad (3.4)$$

Where the indices 1, 2, 3 denote the successive regions, beginning with the Central slab.

Let us write the general solutions (1.2) of the Boltzmann equation in a more convenient form

$$\begin{aligned} \Psi_n(x, \mu) = & a_n e^{-\frac{x-\varrho_{n-1}}{l_n^{v_n}}} \Phi_n(\mu, v_n) + b_n e^{\frac{x-\varrho_n}{l_n^{v_n}}} \Phi_n(\mu, -v_n) + \\ & + \int_{-1}^1 \left\{ A_n(v) e^{-\frac{x-\varrho_{n-1}}{l_n^v}} x(v) + B_n(-v) e^{-\frac{x-\varrho_n}{l_n^v}} x(-v) \right\} \Phi_n(\mu, v) dv \end{aligned} \quad (3.5)$$

$$\text{for } n = 1, 2$$

$$\begin{aligned} \Psi_3(x, \mu) = & a_3 e^{-\frac{x-\varrho_2}{l_3^{v_3}}} \Phi_3(\mu, v_3) + b_3 e^{\frac{x-\varrho_3}{l_3^{v_3}}} \Phi_3(\mu, -v_3) \\ & + \int_{-1}^1 \{A_3(v)\chi(v) + B_3(-v)\} e^{-\frac{x-\varrho_3}{l_3^v}} \Phi_3(\mu, v) dv \end{aligned} \quad (3.6)$$

where

$$\chi(v) = \begin{cases} 1 & \text{for } v > 0 \\ 0 & \text{for } v < 0 \end{cases} \quad (3.7)$$

As the conditions (3.1) and (3.4) are identical with the similar condition in the Chapter

If the solution can be readily obtained in the form

$$A_1(v) = e^{-\frac{d_1}{v}} B_1(v) \quad (3.1)$$

$$a_1 = e^{-\frac{d_1}{v_1}} b_1 \quad (3.2)$$

where

$$d_1 = \frac{q_1}{l_1} \quad (3.10)$$

and

$$B_3(v) = 0 \quad (3.11)$$

$$b_3 = 0 \quad (3.12)$$

Multiplying both sides of Eqs (3.2) and (3.3) by $\mu\Phi_2(\mu, v)$ and $\mu\Phi_2(\mu, \pm v_2)$, respectively and integrating over $\mu \in (-1, 1)$ we obtain the system of equations:

$$vN_{22}(v) \left\{ A_2(v) \chi(v) + B_2(-v) e^{-\frac{d_2}{v}} \chi(-v) \right\} = \int_{-1}^1 \mu \Phi_2(\mu, v) \Psi_1(q_1, \mu) d\mu \quad (3.13)$$

$$vN_{22}(v) \left\{ A_2(v) e^{-\frac{d_2}{v}} \chi(v) + B_2(-v) \right\} = \int_{-1}^1 \mu \Phi_2(\mu, v) \Psi_3(q_2, \mu) d\mu \quad (3.14)$$

$$N_2(v_2) a_2 = \int_{-1}^1 \mu \Phi_2(\mu, v_2) \Psi_1(q_1, \mu) d\mu \quad (3.15)$$

$$N_2(-v_2) e^{-\frac{d_2}{v_2}} b_2 = \int_{-1}^1 \mu \Phi_2(\mu, -v_2) \Psi_1(q_1, \mu) d\mu \quad (3.16)$$

$$N_2(v_2) e^{-\frac{d_2}{v_2}} a_2 = \int_{-1}^1 \mu \Phi_2(\mu, v_2) \Psi_3(q_2, \mu) d\mu \quad (3.17)$$

$$N_2(-v_2) b_2 = \int_{-1}^1 \mu \Phi_2(\mu, -v_2) \Psi_3(q_2, \mu) d\mu \quad (3.18)$$

where

$$d_2 = \frac{q_2 - q_1}{l_2} \quad (3.19)$$

Eliminating the expansion coefficients with the index 2 from these equations we can reduce them to the form:

$$e^{-\frac{d_2}{v}} \int_{-1}^1 \mu \Phi_2(\mu, v) \Psi_1(q_1, \mu) d\mu = \int_{-1}^1 \mu \Phi_2(\mu, v) \Psi_3(q_2, \mu) d\mu \quad (3.20)$$

for $v > 0$

$$\int_{-1}^1 \mu \Phi_2(\mu, -\nu) \Psi_1(\varrho_1, \mu) d\mu = e^{-\frac{d_2}{\nu}} \int_{-1}^1 \mu \Phi_2(\mu, -\nu) \Psi_3(\varrho_2, \mu) d\mu \quad (3.21)$$

for $\nu > 0$

$$e^{-\frac{d_2}{\nu}} \int_{-1}^1 \mu \Phi_2(\mu, \pm \nu_2) \Psi_1(\varrho_1, \mu) d\mu = \int_{-1}^1 \mu \Phi_2(\mu, \pm \nu_2) \Psi_3(\varrho_2, \mu) d\mu \quad (3.22)$$

With the "orthogonality" relations of Chapter I we have.

$$\int_{-1}^1 \mu \Phi_2(\mu, \nu) \Psi_3(\varrho_2, \mu) d\mu = \nu N_{23}(\nu) A_3(\nu) + \frac{c_3 - c_2}{2} \nu \int_0^1 \frac{\mu A_3(\mu)}{\mu - \nu} d\mu + a_3 \nu \frac{c_3 - c_2}{c_3} \Phi_3(\nu, \nu_3) \quad (3.23)$$

Using Eq. (3.23), the Eq. (3.20) has a form

$$N_{23}(\nu) A_3(\nu) + \frac{c_3 - c_2}{2} \int_{-1}^1 \frac{\mu A_3(\mu)}{\mu - \nu} d\mu = -\frac{e^{-\frac{d_2}{\nu}}}{\nu} \int_{-1}^1 \mu \Phi_2(\mu, \nu) \Psi_1(\varrho_1, \mu) d\mu - a_3 \frac{c_3 - c_2}{c_3} \Phi_3(\nu, \nu_3) \quad (3.24)$$

This equation is solved in App. A. The solution has a form

$$A_3(\nu) = \hat{K}_{23} \left\{ -\frac{e^{-\frac{d_2}{\nu}}}{\nu} \int_{-1}^1 \mu \Phi_2(\mu, \nu) \Psi_1(\varrho_1, \mu) d\mu - a_3 \frac{c_3 - c_2}{c_3} \Phi_3(\nu, \nu_3) \right\} \quad (3.25)$$

where the operator \hat{K}_{23} is defined by Eq. (A. 25). Similarly as in the Eq. (3.23) we have

$$\int_{-1}^1 \mu \Phi_2(\mu_1 - \nu) \Psi_3(\varrho_2, \mu) d\mu = -\frac{c_3 - c_2}{2} \int_0^1 \frac{\mu A_3(\mu)}{\mu + \nu} d\mu \quad (3.26)$$

for $\nu > 0$

which with the Eqs (3.11) and (3.25) gives

$$\begin{aligned} & \int_{-1}^1 \mu \Phi_2(\mu, -\nu) \Psi_3(\varrho_2, \mu) d\mu \\ &= -\frac{c_3 - c_2}{2} \nu e^{-\frac{d_2}{\nu}} \int_0^1 \frac{\mu d\mu}{\mu + \nu} \left[\hat{K}_{23} \left\{ e^{-\frac{d_2}{\mu}} \int_{-1}^1 \eta \Phi_2(\eta, \mu) \Psi_1(\varrho_1, \eta) d\eta + a_3 \frac{c_3 - c_2}{c_3} \Phi_3(\mu, \nu_3) \right\} \right] \end{aligned} \quad (3.27)$$

Denoting the term in the function $\Psi_1(\varrho_1, \mu)$ connected with the continuous spectrum by $\Psi_c(\mu)$ the function $\Psi_1(\varrho, \mu)$ can be written as follows

$$\Psi_1(\varrho_1, \mu) = \Psi_c(\mu) + a_1 \Phi_1(\mu, \nu_1) + b_1 e^{-\frac{d_1}{\nu_1}} \Phi_1(\mu, -\nu_1) \quad (3.28)$$

Using Eqs (3.9) and (3.28) we have Eq. (3.27) in the form

$$\int_{-1}^1 \mu \Phi_2(\mu, -v) \Psi_c(\mu) d\mu + \\ + \frac{c_3 - c_2}{2} v e^{-\frac{d_2}{v}} \int_{-1}^3 \frac{\mu d\mu}{\mu + v} \hat{K}_{23} \left\{ \frac{e^{-\frac{d_2}{\mu}}}{\mu} \int_{-1}^1 \eta \Phi_2(\eta, \mu) \Psi_c(\eta) d\eta \right\} = b_1 f(v) + a_3 g(v) \quad (3.29)$$

where

$$f(v) = \frac{c_1 - c_2}{c_1} \left[e^{-\frac{2d_1}{v_1}} \Phi_1(-v, v_1) + \Phi_1(-v, -v_1) + \right. \\ \left. + \frac{c_3 - c_2}{2} v e^{-\frac{d_2}{v}} \int_0^1 \frac{\mu d\mu}{\mu + v} \hat{K}_{23} \left\{ e^{-\frac{d_2}{\mu}} - \left[e^{-\frac{2d_1}{v_1}} \Phi_1(\mu, v_1) + \Phi_1(\mu, -v_1) \right] \right\} \right] \quad (3.30)$$

$$g(v) = \frac{(c_3 - c_2)^2}{2c_3} v e^{-\frac{d_2}{v}} \int_0^1 \frac{\mu d\mu}{\mu + v} \hat{K}_{23} \{ \Phi_3(\mu, v_3) \} \quad (3.31)$$

Similarly, Eq. (3.22) can be expressed by

$$e^{\mp \frac{d_2}{v_2}} \int_{-1}^1 \mu \Phi_2(\mu, \pm v_2) \Psi_1(v_1, \mu) d\mu = \frac{c_2 - c_3}{2} \frac{v_2 v_3}{v_2 \mp v_3} a_3 - \frac{c_2 - c_3}{c_2} \int_0^1 \mu \Phi_3(\mu) \Phi_2(\mu, \pm v_2) d\mu \quad (3.32)$$

Inserting Eq. (3.25) into the last equation we obtain

$$e^{\mp \frac{d_2}{v_2}} \int_{-1}^1 \mu \Phi_2(\mu, \pm v_2) \Psi_1(v_1, \mu) d\mu = \frac{c_2 - c_3}{2} \frac{v_2 v_3}{v_2 \mp v_3} a_3 - \\ - \frac{c_2 - c_3}{c_2} \int_{-1}^1 \mu \Phi_2(\mu, \pm v_2) \hat{K}_{23} \left\{ \frac{e^{-\frac{d_2}{\mu}}}{\mu} \int_{-1}^1 \eta \Phi_2(\eta, \mu) \Psi_1(v_1, \eta) d\eta - a_3 \frac{c_2 - c_3}{c_3} \Phi_3(\mu, v_3) \right\} d\mu \quad (3.33)$$

which can be written also as

$$e^{\mp \frac{d_2}{v_2}} \int_{-1}^1 \mu \Phi_2(\mu, \pm v_2) \Psi_c(\mu) d\mu + \\ + \frac{c_2 - c_3}{c_2} \int_{-1}^1 \mu \Phi_2(\mu, \pm v_2) \hat{K}_{23} \left\{ \frac{e^{-\frac{d_2}{\mu}}}{\mu} \int_{-1}^1 \eta \Phi_2(\eta, \mu) \Psi_c(\eta) d\eta \right\} d\mu = \alpha \pm b + \gamma \pm a_3 \quad (3.34)$$

where

$$\alpha_{\pm} = \mp e^{-\frac{d_2}{v_2} \frac{c_2 - c_1}{2}} \left\{ \frac{v_1 v_2}{v_2 \mp v_1} e^{-\frac{2d_1}{v_1}} + \frac{v_1 v_2}{v_2 \pm v_1} \right\} -$$

$$- \frac{c_2 - c_3}{c_2} \frac{c_1 - c_2}{c_1} \int_0^1 \mu \Phi_2(\mu, \pm v_2) \hat{K}_{23} \left\{ e^{-\frac{d_2}{\mu}} \left[\Phi_1(\mu, v_1) e^{-\frac{2d_1}{v_1}} - \Phi_1(\mu, -v_1) \right] \right\} d\mu \quad (3.35)$$

$$\gamma_{\pm} = \frac{c_2 - c_3}{v_2 \mp v_3} + \frac{[c_2 - c_3]^2}{c_2 c_3} \int_0^1 \mu \Phi_2(\mu, \pm v_2) \hat{K}_{23} \{ \Phi_3(\mu, v_3) \} d\mu \quad (3.36)$$

With the conditions (3.8) Eq. (3.34) can be reduced to

$$\alpha_{\pm} b_1 + \gamma_{\pm} a_3 = \Gamma_{\pm} [B_1(v)] \quad (3.37)$$

where the functionals $\Gamma_{\pm} [B_1(v)]$ are given by

$$\Gamma_{\pm} [B_1(v)] = e^{\mp \frac{d_2}{v_2} \frac{c_2 - c_1}{c_2}} \int_0^1 B_1(v) \left\{ e^{-\frac{2d_1}{v}} \Phi_2(v, \pm v_2) + \Phi_2(-v, \pm v_2) \right\} dv +$$

$$+ \frac{c_2 - c_1}{c_2} \int_0^1 \mu \Phi_2(\mu, \pm v_2) \hat{K}_{23} \left\{ e^{-\frac{d_2}{\mu}} \int_{-1}^1 \eta \Phi_2(\eta, \mu) \int_0^1 B_1(v) \left[e^{-\frac{2d_1}{v}} \Phi_1(\eta, v) + \right. \right.$$

$$\left. \left. + \Phi_1(\eta, -v) \right] dv d\eta \right\} d\mu \quad (3.38)$$

Dividing both sides of Eq. (3.37) by a_3 and denoting

$$Y_1(v) = \frac{B_1(v)}{a_3} \quad (3.39)$$

$$\gamma_1 = \frac{b_1}{a_3} \quad (3.40)$$

we can rewrite it in the form

$$\gamma_1 = \frac{1}{\alpha_{\pm}} \{ \Gamma_{\pm} [Y_1(v)] - \gamma_{\pm} \} \quad (3.41)$$

Comparing the above equations for quantities with plus and minus indices, respectively, we obtain the condition

$$\frac{1}{\alpha_{+}} \{ \Gamma_{+} [Y_1(v)] - \gamma_{+} \} = \frac{1}{\alpha_{-}} \{ \Gamma_{-} [Y_1(v)] - \gamma_{-} \} \quad (3.42)$$

The similar procedure applied to the equation (3.23) gives it in the form

$$N_{21}(v) Y_1(v) + \frac{c_1 - c_2}{2} \int_0^1 \frac{\mu Y_1(\mu)}{\mu - v} d\mu + \int_0^1 \Omega(\mu, v) Y_1(\mu) d\mu = -\frac{1}{v} \left\{ g(v) - \frac{\gamma_{+}}{\alpha_{+}} f(v) \right\} \quad (3.43)$$

where

$$\begin{aligned} & \int_{-1}^1 \Omega(\mu, \nu) Y_1(\mu) d\mu = \frac{c_1 - c_2}{2} \int_0^1 \frac{\mu e^{-\frac{2d_1}{\nu}} Y_1(\mu) d\mu}{\nu - \mu} - \frac{\Gamma[Y_1(\mu)] f(\nu)}{\alpha_+ \nu} = \\ & = \frac{c_3 - c_2}{2} e^{-\frac{d_1}{\nu}} \int_0^1 \frac{\mu}{\mu + \nu} \hat{K}_{23} \left\{ e^{-\frac{d_1}{\mu}} \int_0^1 \eta \Phi_2(\eta, \mu) \int_{-1}^1 Y_1(\xi) \left[e^{-\frac{d_2}{\xi}} \Phi_1(\eta, \xi) - \Phi_1(\eta, \xi) \right] d\xi d\eta \right\} d\mu \end{aligned} \quad (3.44)$$

It can be easily seen that the kernel $\Omega(\mu, \nu)$ is a Fredholm type kernel. Therefore Eq. (3.43) can be reduced to the Fredholm equation by treating it with the operator defined by (A.25).

As the index of the singular integral equation (3.43) is equal to zero, the reduction to the Fredholm equation does not involve any additional condition. Therefore the solution of the considered problem is equivalent to the solution of the Fredholm equation

$$Y_1(\nu) + \hat{K}_{21} \left\{ \int_0^1 \Omega(\mu, \nu) Y_1(\mu) d\mu \right\} = -\hat{K}_{21} \left\{ \frac{1}{\nu} \left[g(\nu) - \frac{\gamma_+}{\alpha_+} f(\nu) \right] \right\} \quad (3.45)$$

with the additional condition (3.42) which plays the role of a critical condition.

The approximate method proposed in App. B, can be used in obtaining the solution of this equation.

4. The critical problem of a slab with an finite reflector

Let us consider a system consisting of a central slab of the thickness $2\varrho_1$, characterized by material parameters c_1 and i_1 surrounded by two symmetrical reflectors of the thickness $\varrho_2 - \varrho_1$ described by material parameters c_2 and i_2 . The origin of x -axis in the Cartesian coordinate system lies in the central plane of the slab.

We can solve this problem in two ways. The first one is based on the previous considerations. Putting $c_3 \rightarrow 0$ in the problem considered in Chapter III we obtain the identical system. However, the passing to this limiting case is not trivial because the operator \hat{K}_{23} changes its class so that a new form of the additional conditions is generated. In the second method the system with finite reflector is treated independently from the beginning. In the Chapter II it was showed that both methods of treatment of finite systems are equivalent. In order to avoid tedious algebra in further analysis the second way is chosen.

Using the symmetry properties of considered system the boundary conditions can be written as follows

$$\Psi_1(0, \mu) = \Psi_1(0, -\mu) \quad (4.1)$$

$$\Psi_1(\varrho_1, \mu) = \Psi_2(\varrho_1, \mu) \quad (4.2)$$

and

$$\Psi_2(\varrho_2, \mu) = 0 \quad \text{for} \quad \mu < 0 \quad (4.3)$$

The solution of Boltzmann equation in our case will be taken in the form (3.5).

The condition (4.1) which is identical with the condition (3.1) can be reduced to

$$A_1(\nu) = e^{-\frac{d_1}{\nu}} B_1(\nu) \quad (4.4)$$

and

$$a_1 = e^{-\frac{d_1}{\nu_1}} b_1 \quad (4.5)$$

Let us write the condition (4.3) in the explicit form

$$a_2 e^{-\frac{d_2}{\nu_2}} \Phi_2(-\mu, \nu_2) - b_2 \Phi_2(-\mu, -\nu_2) + \int_0^1 t_2(\nu) e^{-\frac{d_2}{\nu}} \Phi_2(-\mu, \nu) d\nu + \int_0^1 B_2(\nu) \Phi_2(-\mu, -\nu) d\nu = 0 \quad \text{for} \quad \mu > 0 \quad (4.6)$$

Using the properties of the function $\Phi_2(\mu, \nu)$ we can write Eq. (4.6) in the form

$$\lambda_2(\mu) B_2(\mu) - \frac{c_2}{2} \int_0^1 \frac{\nu B_2}{\nu - \mu} d\nu = -\frac{c_2}{2} \int_0^1 \frac{\nu e^{-\frac{d_2}{\nu}} A_2(\nu)}{\nu - \mu} d\nu - a_2 e^{-\frac{d_2}{\nu_2}} \Phi_2(\mu, -\nu_2) - b_2 \Phi_2(\mu, \nu_2) \quad (4.7)$$

The relation (4.7) has a form of the equation discussed in details by K.M. Case [1] and R. Želazny [2].

The solution of this equation has the form:

$$B_2(\mu) = -\hat{K}_2 \left\{ \frac{c_2}{2} \int_0^1 \frac{\nu e^{-\frac{d_2}{\nu}} A_2(\nu)}{\nu - \mu} d\nu + a_2 e^{-\frac{d_2}{\nu_2}} \Phi_2(\mu, -\nu_2) - b_2 \Phi_2(\mu, \nu_2) \right\} \quad (4.8)$$

where the operator \hat{K}_2 can be written as [2]

$$\hat{K}_2 \{f(\mu)\} = \frac{\lambda_2(\mu) f(\mu)}{[\lambda_2(\mu)]^2 + \left[\frac{\pi}{2} c_2 \mu \right]} = -\frac{1}{X_2^-(\mu)} \left[\frac{1}{\lambda_2(\mu) + i \frac{\pi}{2} c_2 \mu} \right] \frac{c_2}{2} \int_0^1 \frac{\eta X_2^-(\eta) f(\eta) d\eta}{\left[\lambda_2(\eta) - i \frac{\pi}{2} c_2 \mu \right] [\eta - \mu]} \quad (4.9)$$

where

$$\bar{\lambda}_2^-(\mu) = e^{-\frac{1}{2} \ln G_2(\mu)} (\mu - 1)^{-1} e^{\frac{1}{2\pi i}} \int_0^1 \frac{\ln G(\eta)}{\eta - \mu} d\eta \quad (4.10)$$

and

$$G_2(\eta) = \frac{\lambda_2(\eta) + i\frac{\pi}{2} c_2 \eta}{\lambda_2(\eta) - i\frac{\pi}{2} c_2 \eta} \quad (4.11)$$

The singular integral equation (4.7) has the index $\kappa = 1$ so that additional condition is generated:

$$\int_0^1 \frac{\eta X_2^-(\eta)}{\lambda_2(\eta) - i\frac{\pi}{2} c_2 \eta} \left\{ a_2 e^{-\frac{d_2}{v_2}} \Phi_2(\eta, -v_2) + b_2 \Phi_2(\eta, v_2) + \frac{c_2}{2} \int_0^1 \frac{e v^{-\frac{d_2}{v}} A_2(v)}{v + \eta} dv \right\} d\eta = 0 \quad (4.12)$$

The condition (4.12) can be rewritten in the form

$$e^{-\frac{d_2}{v_2}} \alpha a_2 + \beta b_2 + \frac{c_2}{2} \int_0^1 v e^{-\frac{d_2}{v}} h(v) A_2(v) dv = 0 \quad (4.13)$$

where

$$\alpha = \int_0^1 \frac{\eta X_2^-(\eta) \Phi_2(\eta, -v_2) d\eta}{\lambda_2(\eta) - \frac{\pi}{2} c_2 i \eta} \quad (4.14)$$

$$\beta = \int_0^1 \frac{\eta X_2^-(\eta) \Phi_2(\eta, v_2) d\eta}{\lambda_2(\eta) - \frac{\pi}{2} c_2 i \eta} \quad (4.15)$$

and

$$h(v) = \int_0^1 \frac{\eta X_2^-(\eta) d\eta}{\left[\lambda_2(\eta) - \frac{\pi}{2} c_2 i \eta \right] [\eta + v]} \quad (4.16)$$

From the condition (4.13) we have

$$b_2 = -\frac{\alpha}{\beta} e^{-\frac{d_2}{v_2}} a_2 - \frac{c_2}{2\beta} \int_0^1 v e^{-\frac{d_2}{v}} h(v) A_2(v) dv \quad (4.17)$$

Inserting Eq. (4.17) into Eq. (4.8) we obtain

$$B_2(\mu) = -\hat{K}_2 \left\{ \frac{c_2}{2} \int_0^1 r e^{-\frac{d_2}{r}} A_2(r) \left[\frac{1}{r-\mu} - \frac{h(r)}{\beta} \Phi_2(\mu, r_2) \right] dv \right\} - \\ - a_2 e^{-\frac{d_2}{r_2}} \hat{K}_2 \left\{ \Phi_2(\mu, -v) - \frac{\alpha}{\beta} \Phi_2(\mu, r_2) \right\} \quad (4.18)$$

Using the formulas (4.17) and (4.18) we can express the function $\Psi_2(\varrho_1, \mu)$ by $A_2(v)$ and a_2 only.

$$\Psi_2(\varrho_1, \mu) = a_2 \Phi_2(\mu, r_2) - e^{-\frac{d_2}{r_2}} \left\{ \alpha e^{-\frac{d_2}{r_2}} + \frac{c_2}{2\beta} \int_0^1 r e^{-\frac{d_2}{r}} h(r) A_2(r) dv \right\} \Phi_2(\mu, -v_2) + \\ + \int_0^1 A_2(v) \Phi_2(\mu, v) dv - \int_0^1 e^{-\frac{d_2}{r}} \Phi_2(\mu, -v) \left[a_2 e^{-\frac{d_2}{r_2}} \hat{K}_2 \left\{ \Phi_2(r, -v_2) - \frac{\alpha}{\beta} \Phi_2(v, r_2) \right\} + \right. \\ \left. - \frac{c_2}{2} \hat{K}_2 \left\{ \int_0^1 r e^{-\frac{d_2}{r}} A_2(r) \left[\frac{1}{r-\mu} - \frac{h(r)}{\beta} \Phi_2(r, r_2) \right] dv \right\} \right] dv \quad (4.19)$$

The last expression may be written as follows

$$\Psi_2(\varrho_1, \mu) = a_2 \bar{\Phi}(\mu) + \int_0^1 A_2(v) \Phi_2(\mu, v) dv + \int_0^1 Q(\mu, v) A_2(v) dv \quad (4.20)$$

where

$$\bar{\Phi}(\mu) = \Phi_2(\mu, r_2) - \frac{\alpha}{\beta} e^{-\frac{2d_2}{r_2}} \Phi_2(\mu, -v_2) - e^{-\frac{d_2}{r_2}} \int_0^1 r e^{-\frac{d_2}{r}} \Phi_2(\mu, -v) \hat{K}_2 \left\{ \Phi_2(r, -v_2) - \right. \\ \left. - \frac{\alpha}{\beta} \Phi_2(v, r_2) \right\} dv \quad (4.21)$$

and

$$\int_0^1 Q(\mu, v) A_2(v) dv = \frac{c_2}{2\beta} \int_0^1 \Phi_2(\mu, -v_2) h(v) v e^{-\frac{d_2}{v}} A_2(v) dv - \\ - \frac{c_2}{2} \int_0^1 e^{-\frac{d_2}{v}} \hat{K}_2 \left\{ \int_0^1 r e^{-\frac{d_2}{r}} A_2(r) \left[\frac{1}{r+\eta} - \frac{h(r)}{\beta} \Phi_2(r, r_2) \right] dv \right\} \Phi_2(\mu, -v) dv \quad (4.22)$$

It can be easily seen that the kernel $Q(\mu, v)$ is of the Fredholm type. Multiplying both sides of Eq. (4.2) by the functions $\mu \Phi_1(\mu, v)$ and $\mu \Phi_1(\mu, \pm v_1)$ respectively, and integrating

over $\mu \in (-1, 1)$ we obtain the system of equations

$$v_1 N_{11}(v) e^{-\frac{d_1}{v}} A_1(v) = \int_{-1}^1 \mu \Phi_1(\mu, v) \Psi_2(\varrho_1, \mu) d\mu \quad (4.23)$$

for $v > 0$

$$-v N_{11}(v) B_1(v) = \int_{-1}^1 \mu \Phi_1(\mu, -v) \Psi_2(\varrho_1, \mu) d\mu \quad (4.24)$$

for $v > 0$

$$N_1(v_1) a_1 = \int_{-1}^1 \mu \Phi_1(\mu, v_1) \Psi_2(\varrho_1, \mu) d\mu \quad (4.25)$$

$$-N_1(v_1) e^{-\frac{d_1}{v_1}} b_1 = \int_{-1}^1 \mu \Phi_1(\mu, -v_1) \Psi_2(\varrho_1, \mu) d\mu \quad (4.26)$$

Using the above relations we can derive from Eqs (4.4) and (4.5) the following equations

$$\int_{-1}^1 \mu \Phi_1(\mu, v) \Psi_2(\varrho_1, \mu) d\mu = -e^{-\frac{2d_1}{v}} \int_{-1}^1 \mu \Phi_1(\mu, -v) \Psi_2(\varrho_1, \mu) d\mu \quad (4.27)$$

for $v > 0$

and

$$\int_{-1}^1 \mu \Phi_1(\mu, v_1) \Psi_2(\varrho_1, \mu) d\mu = -e^{\frac{2d_1}{v_1}} \int_{-1}^1 \mu \Phi_1(\mu, -v_1) \Psi_2(\varrho_1, \mu) d\mu \quad (4.28)$$

With Eq. (4.21) the last two equations can be written as follows

$$\begin{aligned} a_2 \int_{-1}^1 \mu \Phi_1(\mu, v) \Phi(\mu) d\mu &+ \int_0^1 v A_2(v) \frac{c_1 - c_2}{c_1} \Phi_1(v, v_1) dv \cdot \int_0^1 A_2(v) \int_{-1}^1 \mu \Phi_1(\mu, v_1) Q(v, \mu) d\mu dv \\ &- e^{-\frac{2d_1}{v_1}} \left\{ a_2 \int_{-1}^1 \mu \Phi_1(\mu, -v_1) \Phi(\mu) d\mu + \int_0^1 v A_2(v) \frac{c_1 - c_2}{c_1} \Phi_1(v, -v_1) dv \right. \\ &\left. + \int_0^1 A_2(v) \int_{-1}^1 \mu \Phi_1(\mu, -v_1) Q(v, \mu) d\mu dv \right\} \end{aligned} \quad (4.29)$$

and

$$\begin{aligned} a_2 \int_{-1}^1 \mu \Phi_1(\mu, v) \bar{\Phi}(\mu) d\mu &+ \int_{-1}^1 \mu \Phi_1(\mu, v) \int_0^1 A_2(\eta) \Phi_2(\mu, \eta) d\eta \cdot \int_0^1 A_2(v) \int_{-1}^1 \mu \Phi_1(\mu, v) Q(v, \mu) d\mu dv \\ &- e^{\frac{2d_1}{v}} \left\{ a_2 \int_{-1}^1 \mu \Phi_1(\mu, -v) \bar{\Phi}(\mu) d\mu + \int_{-1}^1 \mu \Phi_1(\mu, -v) \int_0^1 A_2(\eta) \Phi_2(\mu, \eta) d\eta \right. \\ &\left. + \int_0^1 A_2(v) \int_{-1}^1 \mu \Phi_1(\mu, -v) Q(v, \mu) d\mu dv \right\} \end{aligned} \quad (4.30)$$

for $v > 0$

Dividing the both sides of Eq. (4.29) and (4.30) by a_2 and using the "orthogonality" properties of the function $\Phi_l(\mu, \nu)$ $l=1, 2$ we obtain Eqs (4.29) and (4.30) in the form

$$\begin{aligned} & \int_0^1 Y_2(\nu) \left[\frac{c_1 - c_2}{2} \nu (\Phi_1(\nu, \nu_1) + e^{-\frac{2d_1}{\nu_1}} \Phi_1(\nu, -\nu_1)) + \right. \\ & \left. + \int_{-1}^1 \mu Q(\nu, \mu) \left(\Phi_1(\mu, \nu_1) + e^{-\frac{2d_1}{\nu_1}} \Phi_1(\mu, -\nu_1) \right) d\mu \right] d\nu \\ & = \int_{-1}^1 \mu \bar{\Phi}(\mu) \left(\Phi_1(\mu, \nu_1) + e^{-\frac{2d_1}{\nu_1}} \Phi_1(\mu, -\nu_1) \right) d\mu \end{aligned} \quad (4.31)$$

and

$$\begin{aligned} & \nu N_{21}(\nu) Y_2(\nu) + \frac{c_2 - c_1}{2} \nu \int_0^1 \frac{\mu Y_2(\mu)}{\mu - \nu} d\mu + \frac{c_2 - c_1}{2} \nu \int_0^1 \frac{\mu Y_2(\mu) e^{-\frac{d_1}{\nu}}}{\mu + \nu} d\mu + \\ & + \int_0^1 Y_2(\eta) \int_{-1}^1 (\mu Q(\eta, \mu) \left[\Phi_1(\mu, \nu) + e^{-\frac{2d_1}{\nu}} \Phi_1(\mu, -\nu) \right] d\mu d\eta \\ & = - \int_{-1}^1 \mu \bar{\Phi}(\mu) \left[\Phi_1(\mu, \nu) + e^{-\frac{2d_1}{\nu}} \Phi_1(\mu, -\nu) \right] d\mu d\eta \end{aligned} \quad (4.32)$$

where

$$Y_2(\mu) = \frac{A_2(\mu)}{a_2} \quad (4.33)$$

Eq. (4.32) can be rewritten in the form

$$\begin{aligned} & N_{12}(\nu) Y_2(\nu) + \frac{c_1 - c_2}{2} \int_0^1 \frac{\mu Y_2(\mu)}{\mu - \nu} d\mu + \int_{-1}^1 \Omega(\mu, \nu) Y_2(\mu) d\mu \\ & = - \frac{1}{\nu} \int_{-1}^1 \mu \bar{\Phi}(\mu) \left[\Phi_1(\mu, \nu) + e^{-\frac{2d_1}{\nu}} \Phi_1(\mu, -\nu) \right] d\mu \end{aligned} \quad (4.34)$$

where

$$\Omega(\mu, \nu) = \frac{c_2 - c_1}{2} \frac{\mu e^{-\frac{2d_1}{\nu}}}{\nu + \mu} + \frac{1}{\nu} \int_{-1}^1 \eta Q(\mu, \eta) \left[\Phi_1(\eta, \nu) + e^{-\frac{2d_1}{\nu}} \Phi_1(\eta, -\nu) \right] d\eta \quad (4.35)$$

This is the singular integral equation the dominant part of which is identical with the equation considered in App. A. Using the operator \hat{K}_{21} we can reduce Eq. (4.35) to the

Fredholm equation of the form:

$$Y_2(\nu) + \hat{K}_{21} \left\{ \int_0^1 \Omega(\mu, \nu) Y_2(\mu) d\mu \right\} \\ = \hat{K}_{21} \left\{ \frac{1}{\nu} \int_0^1 \mu \bar{\Phi}(\mu) \left[\Phi_1(\mu, \nu) + e^{-\frac{2d_1}{\nu}} \Phi_1(\mu, -\nu) \right] d\mu \right\} \quad (4.36)$$

without any additional condition.

So the equation (4.36) together with the critical condition (4.31) uniquely determines the solution of Boltzmann equation.

It is clear that method of approximate solution proposed in the App. B as well as other approximate methods can be used in this case, too.

5. Conclusions

In the report the following critical problems been considered:

- a) multiplying slab with infinite reflector
- b) three-zone core with infinite reflector
- c) slab with finite reflector.

The solutions of all this problems have been reduced to the solution of the one Fredholm integral equation with the additional critical condition. The solutions of respective Fredholm equations are not known in analytical form.

However, the approximate numerical procedures can be used. Such a procedure involving the spherical harmonics representation has been proposed.

The proposed spherical harmonics method is different from the classical one in the point that only the transport part of the solution is expanded into spherical harmonics.

It is worth to note that in all considered problems the same form of the operators \hat{K}_{lm} and the functions $X_{lm}^-(\mu)$ is met. Therefore the operators and the functions can be tabulated independently what the problem is considered.

The generalization of the method for the systems with the greater number of layers on for the non-symmetrical systems should not lead to the basic difficulties. The increase of the number of layers gives only the increasing of the number of resulting Fredholm equations.

For instance, the solution for the three-zone reactor with finite reflectors can be reduced to the solution of the system of two Fredholm equation with one additional condition.

In all considerations it was facility assumed the none of the c_l 's is equal to the unity. However, when one of c_l tends to the unity, the discrete eigenfunctions tend to the form given e.g. by Van Kampen [4] all results are still valid.

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APPENDIX A

Reduction of the singular integral equation to the Fredholm type

The general theory of singular integral equations given by N. I. Muskhelishvili [3] can be used in solving the equation of the type

$$Q(\mu)Y(\mu) - \frac{1}{\pi i} \int_0^1 \frac{\mathcal{P}(\nu)Y(\nu)}{\nu - \mu} d\nu = f(\mu) \quad (\text{A.1})$$

where

$$Q(\mu) = \lambda_l(\mu)\lambda_k(\mu) + \frac{\pi}{4} c_l c_k \mu^2 \quad (\text{A.2})$$

and

$$\mathcal{P}(\mu) = -\frac{c_l - c_k}{2} \pi i \mu \quad (\text{A.3})$$

According to Muskhelishvili's method we introduce a sectionally holomorphic function.

$$N(z) \stackrel{\text{def}}{=} \frac{1}{2\pi i} \int \frac{\mathcal{P}(\nu)Y(\nu)}{\nu - z} d\nu \quad (\text{A.4})$$

Using Plenely formulas we obtain from Eq. (A. 1).

$$[Q(\mu) - \mathcal{P}(\mu)]N^+(\mu) - [Q(\mu) + \mathcal{P}(\mu)]N^-(\mu) = \mathcal{P}(\mu)f(\mu) \quad (\text{A.5})$$

Where $N^+(\mu)$ and $N^-(\mu)$ denote the limiting values of the function $N(z)$ when z tend to the cut $(0,1)$ from right and left side, respectively. We can rewrite Eq. (A.5) in the form

$$G(\mu)N^+(\mu) - N^-(\mu) = g(\mu) \quad (\text{A.6})$$

where

$$G(\mu) = \frac{Q(\mu) - \mathcal{P}(\mu)}{Q(\mu) + \mathcal{P}(\mu)} \quad (\text{A.7})$$

and

$$g(\mu) = \frac{\mathcal{P}(\mu)f(\mu)}{Q(\mu) + \mathcal{P}(\mu)} \quad (\text{A.8})$$

The function $N(z)$ defined by Eq. (A.4) has the following properties:

a) $N(z)$ is analytic in the complex plane with cut from 0 to 1.

b) $N(z)$ is vanishing at infinity as $\frac{1}{z}$

c) $N(z)$ is bounded by $\frac{c}{z^\alpha}$ and $\frac{c}{(1-z)^\alpha}$ with $\alpha < 1$ as $z \rightarrow 0$ and $z \rightarrow 1$, respectively.

Now the problem of solving Eq. (A.1) is reduced to the solution of the Hilbert problem (A.6) with the additional conditions (a), (b) and (c).

It is easily seen that the function $X_{lk}(z)$ defined by the equation

$$X_{lk}(z) = e^{\frac{1}{2\pi i} \int_0^1 \frac{\ln G(\mu)}{\mu - z} d\mu} \quad (\text{A.9})$$

is a certain solution of the homogeneous Hilbert problem that is of Eq. (A.6) with $g(\mu) = 0$.

Let us investigate the behaviour of the function near the ends of the interval (0,1).

It can be easily proved that near the points $z = c_k$ where $c_0 = 0$ and $c_1 = 1$, respectively

$$X_{lk} \approx (z - c_n)^{\alpha u + i\beta u} \Omega(z) \quad (\text{A.10})$$

where

$$\alpha u + i\beta u = (-1)^{n+1} \frac{\ln G(c_n)}{2\pi i} \quad (\text{A.11})$$

and $\Omega(z)$ is bounded and nonvanishing at the point c_n . From the definition $G(\mu)$ for $\mu \in (0,1)$

$$\ln G(\mu) = \ln \frac{Q(\mu) - \mathcal{P}(\mu)}{Q(\mu) + \mathcal{P}(\mu)} = 2i\Theta(\mu) \quad (\text{A.12})$$

where

$$\Theta(\mu) = \arg [Q(\mu) - \mathcal{P}(\mu)] \quad (\text{A.13})$$

It gives

$$\ln G(0) = \ln G(1) = 0 \quad (\text{A.14})$$

Hence we obtain that

$$\alpha_0 = \alpha_1 = \beta_0 = \beta_1 = 0 \quad (\text{A.15})$$

and the index of the singular integral equation (A.1) \varkappa is equal to zero

$$\varkappa = \alpha_0 + \alpha_1 = 0 \quad (\text{A.16})$$

So we can conclude that $X_{lk}(z)$ is a bounded function near the points c_n .

Moreover, from the definition of $X_{lk}(z)$ we see that

$$\lim_{z \rightarrow \infty} X_{lk}^{-1} = \text{constant} \neq 0 \quad (\text{A.17})$$

As the function $X_{lk}(z)$ is the solution of the homogeneous Hilbert problem it satisfies the equation

$$\frac{X_{lk}^+(\mu)}{X_{lk}^-(\mu)} = G(\mu) \quad (\text{A.18})$$

Inserting it into Eq. (A.6) we obtain

$$N^+(\mu)X_{lk}^+(\mu) - N^-(\mu)X_{lk}^-(\mu) = g(\mu)X_{lk}^-(\mu) \quad (\text{A.19})$$

Defining a new function

$$M(z) = N(z)X_{lk}(z) \quad (\text{A.20})$$

we can write Eq. (A.19) in the form

$$M^+(\mu) - M^-(\mu) = g(\mu)X_{lk}^+(\mu) \quad (\text{A.21})$$

The general solution of this equation has a form

$$M(z) = \frac{1}{2\pi i} \int_0^1 \frac{g(v)X_{lk}^-(v)}{v-z} dv + \mathcal{P}_n(z) \quad (\text{A.22})$$

where $\mathcal{P}_n(z)$ is an arbitrary polynomial of the n -th degree. Hence we have

$$N(z) = \frac{1}{2\pi i} \frac{1}{X_{lk}(z)} \int_0^1 \frac{g(v)X_{lk}^-(v)}{v-z} dv + \frac{\mathcal{P}_n(z)}{X_{lk}(z)} \quad (\text{A.23})$$

Now we must test whether the function $N(z)$ fulfils the conditions (a), (b) and (c). It can be seen immediately that the conditions (a) and (c) are always satisfied. In order to satisfy the condition (b) we must put

$$\mathcal{P}_n(z) \equiv 0 \quad (\text{A.24})$$

Using Eqs. (A.4), (A.23), (A.24) and Plemely formulas we obtain the solution of the singular integral equation (A.1) in the form

$$Y(\mu) = \check{K}_{lk}\{f(\mu)\} = \frac{Q(\mu)}{Q^2(\mu) - \mathcal{P}^2(\mu)} f(\mu) + \\ - \frac{1}{\pi i} \frac{[Q(\mu) - \mathcal{P}(\mu)]^{-1}}{X_{lk}^-(\mu)} \int_0^1 \frac{X_{lk}^-(v)\mathcal{P}(v)f(v)}{[Q(v) + \mathcal{P}(v)][v-\mu]} dv \quad (\text{A.25})$$

Now if we put $f(\mu)$ in Eq. (A.25) in the form

$$f(\mu) = - \frac{c_l - c_k}{c_l} \left\{ \Phi_2(\mu, -v_l) e^{-\frac{e}{l v_l}} + \Phi_l(\mu, v_l) e^{\frac{e}{l v_l}} - \frac{c_l - c_k}{2} \int_0^1 \frac{v e^{-\frac{2e}{l v}} Y(v)}{v + \mu} dv \right\} \quad (\text{A.26})$$

we obtain the Fredholm type equation for the function $Y(\mu)$.

APPENDIX B

The method of evaluation of the Fredholm integral equation (2.21) and of the critical condition (2.21)

Let us write the Fredholm equation (2.24) in the form

$$Y(\mu) - \int_0^1 e^{-\frac{2p}{lv}} K(v, \mu) Y(v) dv = e^{-\frac{e}{l v_1}} f_1(\mu) + e^{-\frac{e}{l v_1}} f_2(\mu) \quad (\text{B.1})$$

$$K(v, \mu) = \frac{c_1 - c_2}{2T(\mu)} v \left\{ \frac{c_1 - c_2}{2} \int_0^1 \frac{\eta H(\eta) d\eta}{(\eta - \mu)(\eta - v)} - \frac{S(\mu)T(\mu)}{v - \mu} \right\} \quad (\text{B.2})$$

$$f_1(\mu) = \frac{c_1 - c_2}{c_1} S(\mu) \Phi_1(\mu, -v_1) - \frac{[c_1 - c_2]^2}{2c_1 T(\mu)} \int_0^1 \frac{\eta H(\eta) \Phi_1(\eta - v_1)}{\eta - \mu} d\eta \quad (\text{B.3})$$

and

$$f_2(\mu) = \frac{c_1 - c_2}{c_1} S(\mu) \Phi_1(\mu, v_1) - \frac{[c_1 - c_2]^2}{2c_1 T(\mu)} \int_0^1 \frac{\eta H(\eta) \Phi_2(\eta - v_1)}{\eta - \mu} d\eta \quad (\text{B.4})$$

Eq. (B.1) can be written in the spherical representation. Using P_N -approximation we have

$$y_n = \sum_{m=0}^N K_{mn} y_m = e^{-\frac{v}{l_1 v_1}} g_n^1 + e^{\frac{v}{l_1 v_1}} g_n^2 \quad (\text{B.5})$$

where

$$Y(\mu) = \sum_{m=0}^N y_m \mathcal{D}_m(2\mu - 1) \quad (\text{B.6})$$

$$f_1(\mu) = \sum_{m=0}^N g_m^1 \mathcal{D}_m(2\mu - 1) \quad (\text{B.7})$$

$$f_2(\mu) = \sum_{m=0}^N g_m^2 \mathcal{D}_m(2\mu - 1) \quad (\text{B.8})$$

and

$$\begin{aligned} K_{mn}(\varrho) &= (2n+1) \int_0^1 \int_0^1 e^{-\frac{2\varrho}{l_1 v}} K(v, \mu) \mathcal{D}_m(2v-1) \mathcal{D}_n(2\mu-1) d\mu dv \\ &= (2n+1) \int_0^1 e^{-\frac{2\varrho}{l_1 v}} \mathcal{D}_m(2v-1) dv \int_0^1 K(v, \mu) \mathcal{D}_n(2\mu-1) d\mu \end{aligned} \quad (\text{B.9})$$

Eq. (B.5) can be written in the form

$$\|\delta_{mn} - K_{mn}(\varrho)\| \|y_m\| = \left\| e^{-\frac{\varrho}{l_1 v_1}} g_n^1 + e^{\frac{\varrho}{l_1 v_1}} g_n^2 \right\| \quad (\text{B.10})$$

The solution of this equation has a form

$$\|y_m\| = \|\delta_{mn} - K_{mn}(\varrho)\|^{-1} \left\| e^{-\frac{\varrho}{l_1 v_1}} g_n^1 + e^{\frac{\varrho}{l_1 v_1}} g_n^2 \right\| \quad (\text{B.11})$$

Hence ultimately the function $Y(\mu)$

$$Y(\mu) = \left\| e^{-\frac{\varrho}{l_1 v_1}} g_n^1 + e^{\frac{\varrho}{l_1 v_1}} g_n^2 \right\|^T \{ \|\delta_{mn} - K_{mn}(\varrho)\|^{-1} \}^T |\mathcal{D}_m(2\mu-1)| \quad (\text{B.12})$$

Where $\|a_{mn}\|^T$ denotes the transposed matrix.

Finally the critical condition (2.4) has the following form

$$\left\| e^{-\frac{\varrho}{v_1}} g_n^1 + e^{\frac{\varrho}{lv_1}} g_n^2 \right\|^T \left\{ \|\delta_{nm} - K_{nm}(\varrho)\|^{-1} \right\}^T \left\| \int_0^1 \mathcal{P}_m(2\nu - 1) \left[\frac{\nu}{v_2 - \nu} + \frac{\nu e^{\frac{2\varrho}{lv_1}}}{v_2 + \nu} \right] d\nu \right\|$$

$$\nu_1 \begin{pmatrix} e^{-\frac{\varrho}{lv_1}} & e^{\frac{\varrho}{lv_1}} \\ \nu_1 & \nu_2 \end{pmatrix} \quad (\text{B.13})$$

The transcendental equation (B.13) involves only material parameters of the system considered and the thickness ϱ of the multiplying slab. A similar method can be used to the solution of Eqs. (3.45), (4.36) and of the critical conditional (3.42) (4.31), respectively.

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SUPERSTRUCTURAL ANISOTROPY OF THE SPIN WAVE DISPERSION IN ANTIFERROMAGNETICS. PART I: THEORY

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In a previous paper (*Acta phys. Polon.*, **19**, 759 (1960)) the author presented purely geometrical hypotheses about the anisotropic propagation of spin waves in regular antiferromagnetic superstructures. In the present paper theoretical proofs for the rightness of these hypotheses are given.

The general dispersion law for long spin waves has been derived in a tensor form, starting from the Ziman's (*Proc. phys. Soc.*, **65**, 540 (1952)) relation based on the Holstein-Primakoff approximation. The formulae for all 7 regular superstructures have been obtained, valid for arbitrary values J_n and J_s of exchange integrals between nearest and next nearest neighbours respectively. For the extreme cases ($J_n = 0$ or $J_s = 0$), the dispersion anisotropy caused by the superstructure appears to be very pronounced, in full agreement with above mentioned hypotheses. For the more realistic non-zero values of exchange integrals, the anisotropy is also evident but depends on the ratio J_n/J_s . More complete discussion of the shape of isoenergetic surfaces will be published in the second part of this paper.

The theoretical treatment leads to the prediction of a new phenomenon in antiferromagnetics, namely the anisotropic spin wave dispersion which must be attributed to the monoplanar as well as biplanar type of regular superstructure. It has been shown that the magnetic anisotropy does not affect in principle the phenomenon under consideration.

Some remarks have been given concerning the possibility of occurring of analogous phenomena in other lattices and superstructures.

I. Introduction

The purpose of the present paper is to verify theoretically previous hypotheses of the author concerning possible anisotropic behaviour of spin waves in individual cubic regular superstructures. These 10 hypotheses (see also Sec. 2. C. of the present Chapter) have been formulated on the basis of geometrical considerations in the paper by Cofta (1960c), which will be called here I.

According to the principal thesis of I, in the regular¹ superstructures (excepting the natural ones) the energy of the spin wave depends on its direction. The superstructure-dependence of spin wave propagation has been foreseen for the first time by the author (Cofta 1957) by reason of approximate calculations carried out for a few superstructure only, and disregarding the effects of neighbours more distant than the nearest ones. A note concerning the influence of the second (i.e. next nearest) neighbours has been published some months ago² (Cofta 1960a).

In Sec. I. 1 the scope of our theory is determined; in Sec. I. 2 the possible origins of anisotropic propagation of spin waves are shortly written down. The dispersion relation obtained previously in the harmonic oscillator approximation is adopted to our purpose in Ch. II; from the use of power series expansion of the spin operators is justified (Sec. II. 2) and general formulas for the anisotropic dispersion tensor are derived (Sec. II. 3). Some general conclusions deduced from these formulas are given in Sec. III. 1; the results of detailed calculations are presented in Sec. III. 2 for the case of isotropic superstructures and in Sec. III. 3 for the interesting case of the anisotropic ones. In Sec. IV. 1 all the results are summarized. Some additional remarks are given in Sec. IV. 2. In the Appendix I the use of an ϵ -function $B(k)$ is justified in App. II the identity of semi-classical and Ziman's results is shown and in App. III the applicability of the power series expansion of the energy is discussed.

I. 1. Restrictions and assumptions

The subject of our interest are the single domain monocrystals represented by the ideal antiferromagnetic translation lattice (i.e. Bravais lattices) of equal ions. We consider here only those lattices which are composed of two identical interpenetrating ferromagnetic sublattices, the magnetization of each being antiparallel to the other one. The magnetic moments are assumed to be in practice the spin moments, localized in lattice points and coupled by the isotropic exchange interactions of the form

$$\mathcal{H} = -2 \sum_i \sum_j J_{ij} \hat{\mathbf{S}}_i \hat{\mathbf{S}}_j \quad (1)$$

where $\hbar \hat{\mathbf{S}}_i$ is the operator of spin angular momentum at the i -th lattice site, the summation being extended over all the pairs of spins. In other words, we suppose the Heisenberg-Dirac Hamiltonian, involving the direct as well as all types of indirect exchange interactions which may be written in the form (1) (e.g. the superexchange, see Anderson 1950). Let us call all so generalized coefficients J_{ij} "exchange integrals" and restrict our considerations only to the isotropic ones. This means that we suppose an appropriate high symmetry of the chemical lattice as well as that of the ionic orbitals, excluding all possible causes of directional dependence of the exchange integrals. Moreover, we shall consider solely the

¹ As to the definition, see Cofta (1960c).

² Moreover, a short review concerning the problem of superstructural anisotropy of spin-wave propagation has been published recently (Cofta 1960b).

nearest and the second interactions (i.e. the interactions between the nearest or next nearest neighbours respectively), although the formalism used here permits to include the effects of arbitrarily distant neighbours. We shall neglect the influence of crystal boundaries.

We shall also assume the g -factor to be isotropic and equal for both sublattices. Our considerations will be confined to the cubic lattices only (see Sec. I. 2. A) with regular spin super-structure (see Sec. I. 2. C). Our treatment will be valid in principle for temperatures which are sufficiently low as compared with the Néel point (see Ch. II)

I. 2. Possible origins of anisotropic propagation of spin waves

Obviously, the super-structure is no unique possible origin of anisotropic propagation of the spin waves: other causes may also exist, compensating the considered super-structural effects. Let us comment shortly upon all these origins, as listed below.

A. Anisotropic structure of magnetic lattice

The anisotropic structure of magnetic lattice presents a quite evident cause of anisotropic behaviour of all kinds of the wave motion through the crystal. In the case of spin waves, the anisotropic structure causes the directional effects even in ferromagnetics. In order to eliminate the structural anisotropy, we shall confine ourselves to cubic magnetic structures only.

B. Anisotropic interactions between atomic spins

Many mechanisms may occur, causing this sort of anisotropy. Let us survey below the essential cases of such a type.

a) Multipolar and pseudomultipolar coupling

The dipole-dipole as well as quadrupole-quadrupole interactions caused by the spin-orbit coupling may modify slightly the dispersion law for spin waves even in the ferromagnetic case (Kowalewski 1960). But the anisotropy of that origin amounts to only about 2 percent of the isotropic part of the dispersion law. Supposing that the analogous effects modify the antiferromagnetic dispersion law not more than in the ferromagnetic case, we shall ignore the multipolar interactions in our considerations and assume the Hamiltonian of the form (1).

b) Anisotropic exchange integrals

The exchange integrals may depend on the direction on account of several different causes, namely:

α) when the chemical lattice has lower symmetry than the magnetic one: such a situation may give rise to different indirect interactions at the same distance (a simple two-dimensional example is shown at the Fig. 1)

- β) when asymmetric orbitals of magnetic ions are present; the coplanar orbitals (Goode-
nough and Loeb 1955) may be here a typical example;
 γ) when different sublattices are formed by different ions.

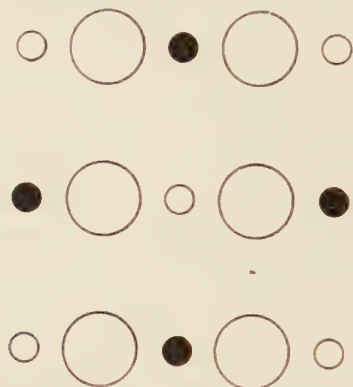


Fig. 1. Example of a chemical lattice in which anisotropy of exchange integral can occur. Large circles symbolize the anions, small — the cations with opposite spins (white and black respectively)

All the mechanisms listed above may cause anisotropy of exchange integrals theoretically even in the ferromagnetic case. The assumptions made in the present paper, eliminate all causes of this art. They will be the subject of future investigation.

C. Anisotropic superstructure

As we have pointed in the paper I, all regular superstructures excepting the natural ones have an anisotropic character. Our restrictions and assumptions admit solely this cause of anisotropy so that all anisotropic effects obtained in our calculations, are only of purely superstructural origin. Let us recall shortly our previous presumptions concerning these effects, presenting them in a tabulated form.

Lattice and superstructure	The expected character of the	
	nearest interactions term	second interactions term
<i>sc</i> —natural	isotropic	isotropic
<i>sc</i> —(001)	(P_1) anisotropic [001]	(P_2) anisotropic [001]
<i>sc</i> —(110)—($\bar{1}\bar{1}0$)	(P_3) anisotropic [001]	(P_4) anisotropic [001]
<i>bcc</i> —natural	isotropic	isotropic
<i>bcc</i> —(110)	(P_5) anisotropic [110] and two other directions	(P_6) anisotropic [001]
<i>fcc</i> —(001)	(P_7) anisotropic [001]	(P_8) isotropic
<i>fcc</i> —(111)	(P_9) anisotropic [111]	(P_{10}) isotropic

Explanation:

We use the notation of regular superstructures introduced by the author in the paper I. To characterize the anisotropy we have given in each case the preferred direction which should be expected (mentioning of one direction only means the uniaxial anisotropy). The symbols P_n number the hypotheses in our paper I.

The above hypotheses concern only extreme cases i.e. the case of vanishing second neighbours exchange integral (nearest interactions term) or that of vanishing nearest neighbours exchange integral (second interactions term). Suppositions as to the form of the dispersion law for $J_s \neq 0$ and $J_n \neq 0$ simultaneously have not been possible, considering that the resulting effect is no simple superposition of the two special cases mentioned above.

II. Adaptation of the dispersion law

II. 1. The approach used

The interactions between spin waves play practically no role in low temperatures, probably up to the $\frac{1}{2}T_N$. We will develop our theory for this range of temperatures (see also Sec. IV. 2). In attempt to investigate only the propagation phenomena of spin waves without their interactions one another, we have to employ, of course, the harmonic oscillator approximation. There exist several different methods using this approximation: 1° the approach of Holstein and Primakoff, 2° the approach of Dyson (both in the so called "linear" or "free magnons" approximation) and 3° the semiclassical approach. All three methods mentioned above lead to the results which are exactly identical to one another, which was to be expected considering the identity of approximation³. Therefore, each of these three approaches can be equally chosen for our purpose. There are available formulae obtained by the method 1° (Ziman 1952) or by the method 3° (Cofta 1959). Both formulae differ merely in notation. Let us employ here the elegant notation by Ziman.

II. 2. Expansion of Ziman's formula

We shall investigate the phenomenon under consideration only in the absence of applied field. Then, the dispersion law for spin waves in antiferromagnetic regular superstructures has the following form in the notation of Ziman (1952):

$$E(\mathbf{k}) = \sqrt{\{A(\mathbf{k})\}^2 - |B(\mathbf{k})|^2} \quad (2)$$

where

$$A(\mathbf{k}) = g\beta H_A + 2S \sum_{\mathbf{r}} J_{\mathbf{r}} \{\sigma_{\mathbf{r}} - \frac{1}{2}(1 + \sigma_{\mathbf{r}}) \cos \mathbf{k}\mathbf{r}\}$$

$$B(\mathbf{k}) = -S \sum_{\mathbf{r}} J_{\mathbf{r}} (1 - \sigma_{\mathbf{r}}) \exp(i\mathbf{k}\mathbf{r}) \quad (3)$$

³ The above statement holds for ferro-, antiferro- and ferrimagnetics. The identity of results obtained by the methods 1° and 3° for the case being treated here, is shortly discussed in the Appendix II to the present paper. The proof for the more general cases will be published in the subsequent papers. It is to be noted that the first remark concerning this identity (for the case of antiferromagnetic natural superstructures with nearest interactions only) has been published by Kubo in the paper by Nagamiya *et al.* (1955). The identity of results of 1° and 2° for the ferrimagnetic simple lattice with antiparallel spins (antiferromagnetism) has been obtained by J. Morkowski (private communication). This is in agreement with the result of J. Kociński (1960) for the ferrimagnetic case with parallel spins.

Here S denotes the maximal value of the z -component of atomic spin, J_r — the exchange integral between the arbitrary spin and its neighbour in the relative position \mathbf{r} . Furthermore — the E is the energy and \mathbf{k} the propagation vector of the spin wave; β stands for the Bohr magneton and g for the Landé factor. The symbol σ_r has the following property: $\sigma_r = 1$ if the spin at the point \mathbf{r} belongs to the same sublattice as the given spin at the point $\mathbf{r} = 0$; otherwise $\sigma_r = -1$. (That is the Luttinger-Ziman method of description of the regular superstructures). The effects of magnetic anisotropy are taken here into account in the phenomenological manner. H_A being the absolute value of the effective magnetic anisotropy field, directed along the z -axis.

The Ziman's formula holds for all regular superstructures (Cofa 1960c). By reason of our assumptions, the function $B(\mathbf{k})$ is a real one (see Appendix I) and we can drop the symbols of absolute value in (2).

In the temperatures for which the free magnon approximation is valid, only the spin waves with small values of k play the essential role:

$$ka \ll 1 \quad (4)$$

(a being the lattice constant). Therefore, we apply for our purpose an approximate form of the formula (2). Using the Taylor's expansion¹

$$F(\mathbf{k}) = F(0) + \mathbf{k} \cdot \left(\frac{dF}{d\mathbf{k}} \right)_{\mathbf{k}=0} + \frac{1}{2} (\mathbf{k} \odot \mathbf{k}) \cdot \left(\frac{d^2 F}{d\mathbf{k}^2} \right)_{\mathbf{k}=0} + \dots \quad (5)$$

for the function E^2 , we obtain

$$E^2 = C + \mathbf{k} \cdot \mathbf{M} \mathbf{k} + \dots \quad (6)$$

where the constant C denotes

$$C = g\beta H_A (g\beta H_A - 2B_0) \\ B_0 = B(0) = -S \sum_r J_r (1 - \sigma_r) \quad (7)$$

whereas the tensor \mathbf{M} may be expressed in the form

$$\mathbf{M} = S \sum_r J_r (\mathbf{r} \odot \mathbf{r}) \{A_0(1 + \sigma_r) - B_0(1 - \sigma_r)\} \quad (8)$$

with

$$A_0 = g\beta H_A + B_0 \quad (8)$$

It can be easily determined that the third non-vanishing term in (6) i.e. the k^4 term amounts to $\frac{a^2 k^2}{12}$ times the second one. Since on account of (4)

$$\frac{a^2 k^2}{12} \lesssim 10^{-3}$$

¹ To avoid mistakes, we employ here the symbol \odot for the dyadic multiplication of two vectors, and the dot for the scalar multiplication of two tensors of any rank (order). Note, that for any second rank tensor \mathbf{T} and any vector \mathbf{v} the relation $(\mathbf{v} \odot \mathbf{v}) \cdot \mathbf{T} = \mathbf{v} \cdot \mathbf{T} \mathbf{v}$ holds.

we can ignore all higher terms in (6) and write in a very good approximation

$$E \approx \{C + \mathbf{kMk}\}^{\frac{1}{2}} \quad (9)$$

Sometimes the dispersion law for long spin waves in antiferromagnetics is expressed also in another form, namely that arising of the approximate power series expansion of the energy. In our general case we get thus:

$$E(\mathbf{k}) \approx \sqrt{C} + \frac{\mathbf{kMk}}{2\sqrt{C}} \quad (10)$$

The shape of isoenergetic surfaces is, of course, the same for both the forms. Nevertheless, we prefer the form (9) because it is valid without any restrictions as to the values of k except of (4). Due to this fact, this form is convenient for simplified calculations, neglecting the magnetic anisotropy. The form (10), instead, behaves differently, since the infinite Taylor series of E has a limited convergence radius⁵, depending on the magnetic anisotropy field strength (see Appendix III) and, moreover, the approximation (10) (i.e. the dropping of the higher terms) is applicable in a rather more restricted range namely for $ak < 10^{-2}$ provided the usual values of H_A (see also the Appendix III); for example, in very thin antiferromagnetic films this condition is not satisfied. For vanishing magnetic anisotropy ($C = 0$), the form (10) is obviously no longer valid.

II.3. The anisotropy tensor \mathbf{M}

We see from eq. (9) that the anisotropy of the spin wave dispersion is characterized completely by the tensor \mathbf{M} . We will now adapt the formula (8) for the case to be investigated here. Let us denote by J_n the exchange integral between the nearest neighbours, by J_s however that between the second ones. Then, by virtue of assumptions of the Section I.1, we may write:

$$B_0 = -2S(J_n z_n^- + J_s z_s^-) \quad (11)$$

where z_n^- and z_s^- denote the numbers of nearest and second neighbours respectively, having the spins aligned oppositely to the spin at the point $\mathbf{r} = 0$. Moreover, let us introduce the notation

$$\varepsilon_A = g\beta H_A \quad (12)$$

From (11) and (8) we get

$$\mathbf{M} = J_n \sum_{\mathbf{r}}^n G_{\mathbf{r}}(\mathbf{r} \odot \mathbf{r}) + J_s \sum_{\mathbf{r}}^s G_{\mathbf{r}}(\mathbf{r} \odot \mathbf{r}) \quad (13)$$

where we have used the abbreviation

$$G_{\mathbf{r}} = \varepsilon_A + \{\varepsilon_A + 2SB_0\} \sigma_{\mathbf{r}} \quad (14)$$

⁵ or, strictly speaking, the limited convergence ellipsoid.

The symbol \sum^n in (13) is used for the summation over the nearest neighbours only, and \sum^s over the second ones.

In order to verify our hypotheses presented in the paper I let us divide the tensor $\mathbf{M}(J_n, J_s)$ which is a function of J_n and J_s , in three parts:

$$\mathbf{M} = \mathbf{M}^n + \mathbf{M}^s + \mathbf{M}^m \quad (15)$$

defined as follows:

$$\begin{aligned} \mathbf{M}^n &= \mathbf{M}(J_n, 0) \\ \mathbf{M}^s &= \mathbf{M}(0, J_s) \\ \mathbf{M}^m &= \mathbf{M} - \mathbf{M}^n - \mathbf{M}^s \end{aligned} \quad (16)$$

Now, by means of (16) we may treat the \mathbf{k} -dependent part of E^2 as separated into three terms: the "nearest interactions term" $\mathbf{kM}^n\mathbf{k}$, the "second interactions term" $\mathbf{kM}^s\mathbf{k}$ and the "mixed" one: $\mathbf{kM}^m\mathbf{k}$. From (13), (14) and (16) we have:

$$\mathbf{M}^n = J_n \cdot \sum^n (\mathbf{r} \odot \mathbf{r}) \{ \varepsilon_A (1 + \sigma_r) - 4S^2 J_n z_n^- \sigma_r \} \quad (17a)$$

$$\mathbf{M}^s = J_s \sum^s (\mathbf{r} \odot \mathbf{r}) \{ \varepsilon_A (1 + \sigma_r) - 4S^2 J_s z_s^- \sigma_r \} \quad (17b)$$

$$\mathbf{M}^m = -4S^2 J_n J_s \{ z_s^- \sum^n (\mathbf{r} \odot \mathbf{r}) \sigma_r + z_n^- \sum^s (\mathbf{r} \odot \mathbf{r}) \sigma_r \} \quad (17c)$$

III. Results

III. 1. General conclusions

Two general conclusions may be deduced from our formulas. The first one concerns the effects of magnetic anisotropy on the phenomenon investigated here. Coming back to the formula (14), we see that the first part is always isotropic (see also the Section III. 2). In the second one, however, the energy of magnetic anisotropy occurs only as an item of the sum $\varepsilon_A + 2SB_0$. The magnetic anisotropy energy is known to be roughly 100 times smaller⁶ than the exchange energy ε_E (defined below):

$$\varepsilon_A \sim 10^{-2} \varepsilon_E \quad (18)$$

For the case of non-vanishing second interactions we have to define the "exchange energy" in a rather more general sense as usually, say:

$$\varepsilon_E = 4S^2 \{ |J_n| z_n^- + |J_s| z_s^- \} \quad (18')$$

For most antiferromagnetic substances holds: $2SB_0 \sim \varepsilon_E$ so that, generally speaking, in the second part of (14) we can neglect the ε_E in comparison with the exchange term $2SB_0$. Hence, we can conclude that the magnetic anisotropy can play an important role in the investigated

⁶ E. g. for the MnF_2 we get $\varepsilon_A = 2 \cdot 10^{-2} \cdot 2SB_0 \sim 2 \cdot 10^{-2} \varepsilon_E$, see Johnson and Nethercot (1959).

superstructural effects only in the rather exceptional case $2SB_0 \leq \varepsilon_A$ which implies on account of (11), (18) and (18):

$$J_n z_n^- + J_s z_s^- \simeq \{|J_n|z_n^- + |J_s|z_s^-\} \times 10^{-2} \quad (19)$$

In that case ε_A can become the unique factor in both the parts of the formula (14), namely when

$$B_0 \approx 0 \quad (20)$$

We will show in the Part II of this paper for each superstructure separately that (20) is rather not to be expected.

The second conclusion concerns the behaviour of the $E(\mathbf{k})$ when the coordinate system is changed. Let us consider a given lattice with a given superstructure, which is oriented in an other direction than that quoted in the table I. Further let us apply the formula (9) to the rotated lattice. It can be seen that the only difference in the dispersion law in comparison with that for the unrotated lattice is the change of the orientation of quadric surface of tensor \mathbf{M} , the new orientation being consistent with that of the lattice; the essential parameters, however, as well as the constant C remain unchanged. In other words, the dispersion relation does not depend on the relative orientation of spins (and the field H_A) with respect to the whole lattice. Hence, the SH_A as well as S^2 involved in (9) may be treated as the invariants of rotation of coordinate axes. This is obvious when we consider that the approximations used here imply small deviations of spins from their common direction, so that SH_A and S^2 behave as the scalar products of two vectors.

III. 2. The isotropic dispersion

Let us calculate at first the tensor \mathbf{M} for isotropic superstructures i.e. the natural ones. We have, of course, in this case $z_n^- = z_n$ (z_n being the number of all nearest neighbours) and $z_s^- = 0$.

Then from (14) and (11) we find:

$$G_{\mathbf{r}} = \varepsilon_A(1 + \sigma_{\mathbf{r}}) - 4S^2 J_n z_n \sigma_{\mathbf{r}} \quad (21)$$

The definition of natural superstructures implies also $\sigma_{\mathbf{r}} = -1$ for all nearest neighbours and $\sigma_{\mathbf{r}} = 1$ for all the second ones; then the formula (13) yields:

$$\mathbf{M} = 4S^2 J_n^2 z_n \sum (\mathbf{r} \odot \mathbf{r}) + J_s (2\varepsilon_A - 4S^2 J_n z_n) \sum (\mathbf{r} \odot \mathbf{r}) \quad (22)$$

It is easy to evaluate the sum $\sum (\mathbf{r} \odot \mathbf{r})$ for neighbours lying on a sphere with radius r :

$$\sum_{\mathbf{r}} (\mathbf{r} \odot \mathbf{r}) = \frac{1}{3} z r^2 \mathbf{E}. \quad (23)$$

Here z is the number of neighbours lying on the sphere and \mathbf{E} denotes the unit tensor. Therefore, for the case being considered we find

$$\mathbf{k} \cdot \mathbf{M} \mathbf{k} = M k^2 \quad (24)$$

with

$$M = \frac{4}{3} S^2 J_n^2 z_n'^2 + \frac{1}{3} J_s z_s (2\varepsilon_A - 4S^2 J_n z_n) r_s^2 \quad (25)$$

where r_n and r_s denote the radii of nearest and second neighbours spheres respectively, z_s being the number of second neighbours. The result (25) shows that the magnetic anisotropy cannot play decisive role in isotropic dispersion relation, since ε_A is always much smaller than $S^2 |J_n| z_n$. In practice, we can disregard ε_A in expressions for M as well as in that for the constant C :

$$C = g\beta H_A (g\beta H_A + 2B_0) \approx 2g\beta H_A B_0 \quad (26)$$

because for natural superstructures

$$B_0 = -2S J_n z_n \quad (27)$$

and therefore B_0 never vanishes. Hence, for the case of natural superstructures of cubic lattices, the spin waves obey the isotropic dispersion law:

$$E = \sqrt{C} + M k^2 \quad (28)$$

where

$$\begin{aligned} C &= -4\varepsilon_A J_n z_n \\ M &= \frac{4}{3} S^2 J_n z_n (J_n z_n r_n'^2 - J_s z_s r_s'^2) \end{aligned} \quad (29)$$

If $|J_s| \ll |J_n|$, then the relation (28) can be written approximately in the form:

$$E \approx 2\sqrt{J_n z_n} \sqrt{-\varepsilon_A + \frac{1}{3} S^2 J_n z_n r_n'^2 k^2} \quad (30)$$

III. 3. Anisotropic results

We will present now the results of calculations of 6 components of the symmetric tensor \mathbf{M} individually for each of 5 anisotropic superstructures of cubic lattices. The lattice constant will be denoted by a . The figures annexed to the present section show the relative positions of the nearest and second neighbours⁷.

a) The case of *sc*-(001)

From the Fig. 2 we find: $z_n^- = 2$, $z_s^- = 8$; hence $B_0 = -4S(J_n + 4J_s)$. From the formula (17a) we get:

$$\begin{aligned} M_{xx}^n &= M_{yy}^n = 4a^2(\varepsilon_A - 4S^2 J_n) J_n \\ M_{zz}^n &= 16a^2 S^2 J_n^2 \\ M_{xy}^n &= M_{yz}^n = M_{zx}^n = 0 \end{aligned} \quad (31)$$

Considering (13) we find a pronounced uniaxial anisotropy of the nearest interactions term, which may be written in a good approximation as proportional to

$$k_x^2 + k_y^2 - k_z^2 \quad (32)$$

⁷ The more complete illustrations of superstructures may be found in the paper I.

Since the preferred direction is the [001] one, our hypothesis P_1 is hereby fully vindicated theoretically.

Likewise we obtain for the second interactions term:

$$\begin{aligned} M_{xx}^s &= M_{yy}^s = 8a^2 \varepsilon_A J_s \\ M_{zz}^s &= (16a)^2 S^2 J_s^2 \\ M_{xy}^s &= M_{yz}^s = M_{zx}^s = 0 \end{aligned} \quad (33)$$

Since $M_{xx}^s \ll M_{zz}^s$, the direction [001] is very strongly preferred in this case (see also the case of *fcc*-(001) in the section 2*d* of the present Chapter). In this manner the rightness of our hypothesis P_2 is also completely demonstrated.

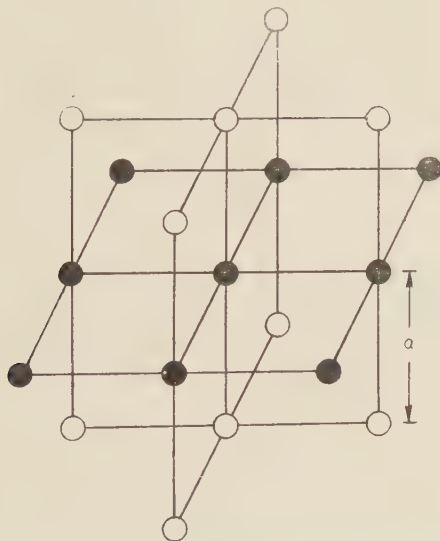


Fig. 2. Relative positions of neighbours in the case of superstructure *sc*-(001)

Taking into account also the mixed term, we get the complete result:

$$\begin{aligned} M_{xx} &= M_{yy} = 4a^2 \{ \varepsilon_A (J_n + 2J_s) - 4S^2 J_n (J_n + 4J_s) \} \\ M_{zz} &= 16a^2 S^2 (J_n + 4J_s)^2 \end{aligned} \quad (34)$$

the non-diagonal components being equal to zero. This result shows also the uniaxial anisotropy with the preferred [001] direction.

b) The case of sc-(110)—(110)

According to Fig. 3 we have: $z_n^- = 4$, $z_s^- = 8$, hence $B_0 = 8S(J_n + 2J_s)$. For the diagonal components of the nearest interactions term we get

$$\begin{aligned} M_{xx}^n &= M_{yy}^n = 32a^2 S^2 J_n^2 \\ M_{zz}^n &= 4a^2 \{ \varepsilon_A - 8S^2 J_n \} J_n \end{aligned} \quad (35)$$

The non-diagonal components vanish. The uniaxial anisotropy, privileging the direction [001] is here evident, in full accord with our prediction P_3 .

The second interactions tensor is also diagonal in this case, with the same direction preferred:

$$\begin{aligned} M_{xx}^s &= M_{yy}^s = 8a^2 \varepsilon_A J_s \\ M_{zz}^s &= 256a^2 S^2 J_s^2 \end{aligned} \quad (36)$$

Similarly with the result (33), here also a strongly pronounced anisotropy occurs, which argues for the reality of our hypothesis P_4 .

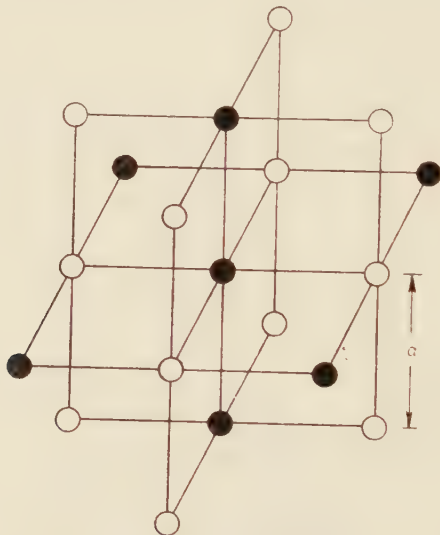


Fig. 3. Relative positions of neighbours in the case of superstructure $sc\text{-(110)}-(\bar{1}\bar{1}0)$

The full result shows the same type of anisotropy as both the special cases given above:

$$\begin{aligned} M_{xx} &= M_{yy} = 8a^2 \{ \varepsilon_A J_s + 4S^2 J_n (J_n + 2J_s) \} \\ M_{zz} &= 4a^2 \{ \varepsilon_A J_n + 8S^2 (4J_s - J_n) (J_n + 2J_s) \} \\ M_{xy} &= M_{yz} = M_{zx} = 0 \end{aligned} \quad (37)$$

Let us emphasize, that for some values of J_n/J_s the effects of nearest and second interactions may be mutually compensated; e.g. when ε_A is disregarded, we obtain for $J_n = 2J_s$ the isotropy of spin wave propagation: $M_{xx} = M_{zz}$.

c) The case of bcc-(110)

As shown at the Fig. 4, we have here $z_n^- = z_s^- = 4$, hence $B_0 = -8S(J_n \perp J_s)$. For the case of nearest interactions only we find:

$$\begin{aligned} M_{xx}^n &= M_{yy}^n = M_{zz}^n = 2a^2 \varepsilon_A J_n \\ M_{xy}^n &= 2a^2 (\varepsilon_A - 16S^2 J_n) J_n \\ M_{yz}^n &= M_{zx}^n = 0 \end{aligned} \quad (38)$$

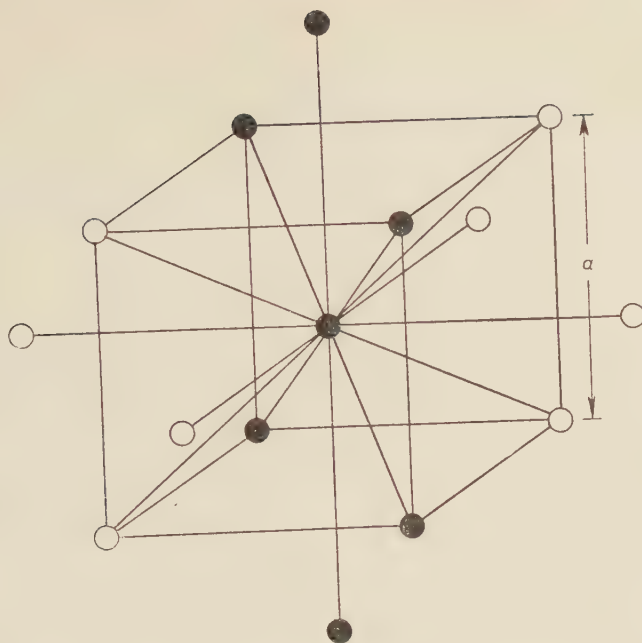


Fig. 4. Relative positions of neighbours in the case of superstructure $bcc-(110)$

In order to show more clearly the anisotropy appearing here, we have to go over to the new cartesian coordinates axes x', y', z' in directions: $[110]$, $[1\bar{1}0]$, and $[001]$ respectively. The appropriate transformation is given by

$$\mathbf{k}' = \mathbf{T}\mathbf{k} \quad (39a)$$

where

$$\mathbf{T} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \quad (39b)$$

In the new coordinates the components of \mathbf{M} are the same as the components of a tensor $\mathbf{M}' = \mathbf{TMT}^{-1}$ in the original system, namely

$$\begin{aligned} (M_{xx}^n)' &= M_{xx}^n - M_{xy}^n = 32a^2 S^2 J_n^2 \\ (M_{yy}^n)' &= M_{xx}^n + M_{xy}^n = 4a^2 J_n (\epsilon_A - 8S^2 J_n) \\ (M_{zz}^n)' &= M_{zz}^n = 2a^2 \epsilon_A J_n \\ (M_{xy}^n)' &= (M_{yz}^n)' = (M_{zx}^n)' = 0 \end{aligned} \quad (40)$$

The result (40) gives proof for the anisotropic behaviour of the nearest interactions term, one of the three favoured directions being perpendicular to the ferromagnetic planes, in full accord with our prediction P_5 .

For the second interactions term we get in the new coordinate system (39):

$$(M_{xx}^s)' = (M_{yy}^s)' = 32a^2 S^2 J_s^2 \quad (41)$$

$$(M_{zz}^s)' = 4a^2 J_s (\epsilon_A - 8S^2 J_s)$$

the other components being equal to zero. The evident uniaxial anisotropy in the [001] direction, which may be seen from (41), gives the theoretical verification of our hypothesis P_6 .

When, moreover the mixed term is taken into account, then the full tensor \mathbf{M} appears also diagonal in the system (39):

$$\begin{aligned} M'_{xx} &= 32a^2 S^2 (J_n - J_s)^2 \\ M'_{yy} &= 32a^2 S^2 (J_s^2 - J_n^2) + 4a^2 \epsilon_A J_n \end{aligned} \quad (42)$$

$$M'_{zz} = -32a^2 S^2 J_s (J_n + J_s) + 2a^2 \epsilon_A (J_n + 2J_s)$$

d) The case of fcc-(001)

From the Fig. 5 we get: $z_n^- = 8$, $z_s^- = 0$; hence $B_0 = -16SJ_n$. The formula for the nearest interactions term gives following components of diagonal tensor \mathbf{M}^n :

$$\begin{aligned} M_{xx}^n &= M_{yy}^n = 2a^2 \epsilon_A J_n \\ M_{zz}^n &= 64a^2 S^2 J_n^2 \end{aligned} \quad (43)$$

As may be seen, this result is in principle identical with both the ones given by (33) and (36). This is no surprise, since the substructure of sc-(001) as well as those of sc-(110)—(110)

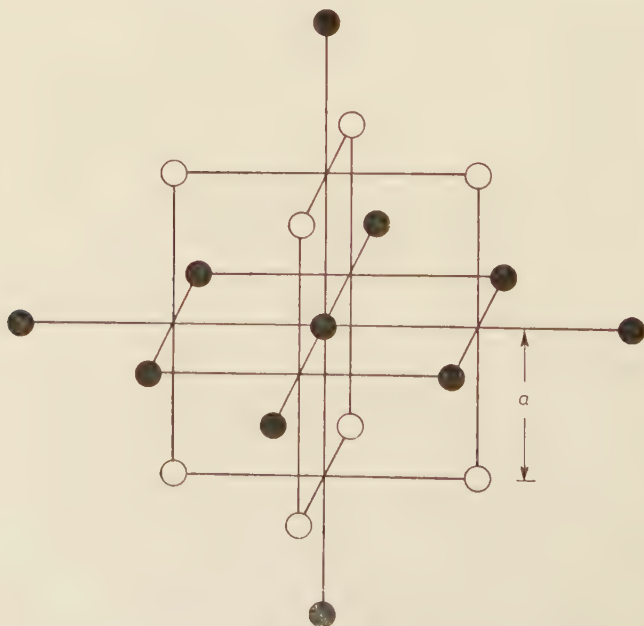


Fig. 5. Relative positions of neighbours in the case of superstructure fcc-(001)

form simply *fcc* lattices with the regular spin ordering (001). The result (43) demonstrates the rightness of the hypothesis P_7 . On the other hand the essential role of the magnetic anisotropy in the components M_{xx} and M_{yy} in (43), (33) and (36), contrasting with its role in the isotropic case, seems rather unexpected. (The result (40) shows also a similar behaviour of M_{zz}).

For the second interactions term our formulae give isotropic result:

$$M_{xx}^s = M_{yy}^s = M_{zz}^s = 4a^2 \varepsilon_A J_s \quad (44)$$

$$M_{xy}^s = M_{yz}^s = M_{zx}^s = 0$$

which corroborates the prediction, formulated in our hypothesis P_8 . It is worth while to note the quite exceptional role of the magnetic anisotropy in (44), which seems to suggest that the exchange interactions of the form (1) between the second neighbours can never be the unique coupling mechanism in the case of superstructure under consideration. Only the simultaneous presence of the nearest and second interactions gives rise to appearing of purely exchange terms in components of the tensor \mathbf{M} (see the result (45) below).

The full expression for \mathbf{M} has the form

$$\begin{aligned} M_{xx} &= M_{yy} = 2a^2 \varepsilon_A (J_n + 2J_s) - 64a^2 S^2 J_n J_s \\ M_{zz} &= 4a^2 \varepsilon_A J_s + 64a^2 S^2 J_n (J_n - J_s) \\ M_{xy} &= M_{yz} = M_{zx} = 0 \end{aligned} \quad (45)$$

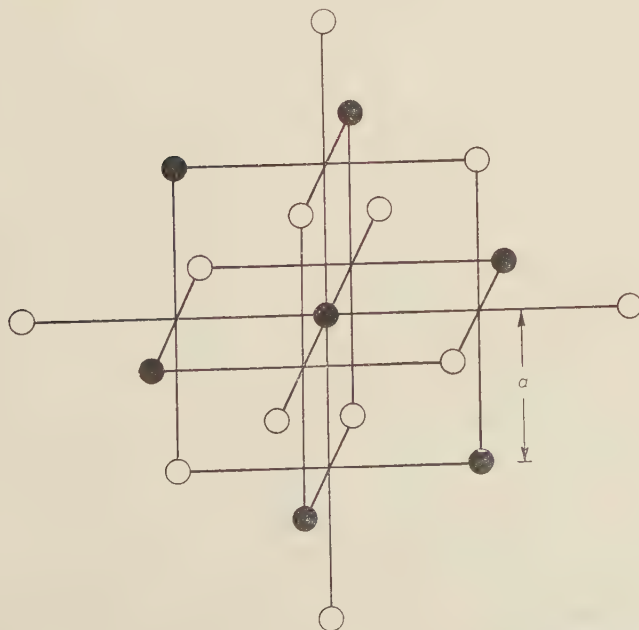


Fig. 6. Relative positions of neighbours in the case of superstructure *fcc*-(111)

e) *The case of fcc-(111)*

In this most interesting case of superstructure we have $z_n^- - z_s^- = 6$ which implies $B_0 = 12S(J_n + J_s)$. The calculations of the sums (17) (see the Fig. 6) give for the nearest interactions term:

$$\begin{aligned} M_{xx}^n &= M_{yy}^n = M_{zz}^n = 2a^2\epsilon_A J_n \\ M_{xy}^n &= M_{yz}^n = M_{zx}^n = a^2 J_n (\epsilon_A + 24S^2 J_n) \end{aligned} \quad (46)$$

In order to show the anisotropic nature of the non-diagonal components we introduce another coordinate axes, the new axis z having the $[111]$ direction in the original system. The two other axes may be chosen quite arbitrarily (provided that they form an orthogonal system), because the anisotropy being considered appears to be an uniaxial one. Let us put the axes x and y in the direction $[11\bar{2}]$ and $[\bar{1}10]$ respectively. Then, using the transformation

$$\mathbf{T} = \frac{1}{\sqrt{6}} \begin{pmatrix} 1 & -\sqrt{3} & \sqrt{2} \\ 1 & \sqrt{3} & \sqrt{2} \\ -2 & 0 & \sqrt{2} \end{pmatrix} \quad (47)$$

we get in the new system:

$$\begin{aligned} (M_{xx}^n)' &= (M_{yy}^n)' = M_{xx}^n - M_{xy}^n = a^2 J_n (\epsilon_A - 24S^2 J_n) \\ (M_{zz}^n)' &= M_{xx}^n + 2M_{xy}^n = 4a^2 J_n (\epsilon_A + 12S^2 J_n) \\ (M_{xy}^n)' &= (M_{yz}^n)' = (M_{zx}^n)' = 0 \end{aligned} \quad (48)$$

This result demonstrates that our predictions, formulated as the hypothesis P_9 , are right.

For the second interactions term we get:

$$M_{xx}^s = M_{yy}^s = M_{zz}^s = 48a^2 S^2 J_s^2 \quad (49)$$

other components being equal to zero. This isotropic result is the theoretical argument for the reasonableness of our hypothesis P_{10} .

The full formulae for the case under consideration are:

$$\begin{aligned} M_{xx}' &= M_{yy}' = a^2 \{ \epsilon_A J_n + 24S^2 (J_n + J_s) (2J_s - J_n) \} \\ M_{zz}' &= 4a^2 \{ \epsilon_A J_n + 12S^2 (J_s + J_n)^2 \} \end{aligned} \quad (50)$$

The isotropic result obtained by Elliot and Lowde (1955) is due to an error⁸ in their calculations.

IV. Conclusions and remarks

IV. 1. Summary of results

In the paper I we have presented on basis of geometrical considerations the 10 hypotheses (see the table in Sec. I. 2. C) concerning possible behaviour of spin waves in the individual 5 regular superstructures for the two extreme cases ($J_s = 0$ or $J_n = 0$). In the

⁸ This isotropy is a consequence of the faulty assumption that in the factor $A - |B|$ the sum over nearest neighbours vanishes.

section *III. 3* of the present paper, we have given the theoretical proofs of the rightness of all these hypotheses in all their details. The superstructural anisotropy of spin wave propagation predicted in $P_1, P_2, P_3, P_4, P_5, P_6, P_7$ and P_9 appears very pronouncedly. The preferred directions agree in all cases with these expected. Also the uniaxial character of the anisotropy is shown for all cases when predicted (i.e. with the exception of P_5). The isotropic dispersion relations expected by P_8 and P_{10} have been proved.

2° It has been supposed that the anisotropy of spin wave propagation will be practically quenched by the energy of magnetic anisotropy. The theoretical calculations presented in the Chapter *III* remove entirely such apprehensions. The existence of magnetic anisotropy does not affect the superstructural phenomena being considered here, except in the case when

$$4S^2|J_n z_n^- + J_s z_s^-| \lesssim \varepsilon_A \quad (51)$$

which seems to be rather impossible for all regular superstructures (a closer examination will be given in the Part II of the present paper). Only in this case the dispersion relation might be the isotropic one, independently of the superstructure.

3° From the formulas obtained in *III. 3* one can get easily all the partial results published in our previous notes, quoted in the Ch. *I*. This holds also for the results obtained by means of the kinematical method (Cofta 1957)⁹

4° From the result (44) we can conclude that in the case of *fcc*-(001), the second interactions play probably an unimportant role.

IV. 2. Final remarks

It is to be noted that the extreme cases investigated here as nearest and second interactions terms respectively, seem to be rather unrealistic. We have calculated these terms solely in order to justify our hypotheses of the paper I.

In practice, neither J_n nor J_s vanishes, and the resulting expression involves both the corresponding terms as well as the mixed one, which has in general a rather complicated form. In consequence, a compensation of nearest and second interactions effects can occur for definite values of J_n and J_s , so that the dispersion relation can become isotropic. Such an effect is possible even when both the interactions favour the same direction as we have seen in *III. 2. b*. We shall analyse accurately the shape of isoenergetic surfaces in the Part II of the present paper, to be published shortly in the A.P.P.

It is to be suggested that also the anharmonic terms in the Hamiltonian must show a kind of the direction-dependence arising from the superstructure. For the same reasons as those presented in the paper I, these higher order directional effects must show, of course, an analogous character (i.e. favouring the same directions) as the ones investigated here. On this ground one can hope that the phenomenon of the superstructural anisotropy may be observed in a larger region of temperatures than that one limited by the free magnons approximation. Moreover, some directional dependence of the resonance line width can be expected for the same reasons.

⁹ As to the equivalence of the kinematical method of Keffer, Kaplan, and Yafet with the other semiclassical ones, see the paper by Cofta (1959).

At the end, let us note some possibilities of extending of present investigations. First of all, the analogous effects i.e. the superstructural dependence of the spin wave propagation, must occur also in the cases of anisotropic interactions. Especially, the case of the anisotropic exchange integrals is an typical domain for such investigations (some results will be given shortly). Further, the superstructural anisotropy of the spin wave dispersion is also possible in the non-translational antiferromagnetic lattices (i.e. in lattices with a basis). Here the effects will be probably weaker than in translational lattices.

Effects similar to these obtained in the present paper will appear also in some kind on non-symmetric superstructures, namely in those in which the ferromagnetic planes exist (excepting the isotropic cases, analogous to the natural cases of the regular superstructure). The approximate calculations for the nearest interactions only lead to the strongest anisotropy possible: the direction perpendicular to the ferromagnetic planes is a "forbidden" one (see also Cofta 1959). Further investigations seem to be very interesting.

The superstructural phenomena must occur obviously also in ferrimagnetic lattices. On account of overlap effects, the character of propagation anisotropy is here surely different from that in antiferromagnetics. The case of ferrimagnetic non-translational lattices is, however, interesting in historical respects. In this most complicated case, the anisotropy of dispersion relation caused by the superstructure has been obtained for the first time, namely by Kouvel (1955) in his excellent spin-wave analysis of magnetite lattice¹⁰. Here the superstructure in *B*-positions causes a weak anisotropy in the [110] direction. If the usual estimations of exchange integrals in spinels are made, this anisotropy amounts to less than 2 percent and therefore seems to be unobservable.

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APPENDIX I

The reality of the function $B(\mathbf{k})$

By virtue of the assumed isotropy of the exchange integrals, we have

$$J_{-\mathbf{r}} = J_{\mathbf{r}} \quad (\text{AI.1})$$

¹⁰ This paper was not known to the author before 1953; this classic work has been, unfortunately, not published as yet. The kindness of Dr Kouvel in sending to the author a copy of his work is greatly appreciated.

Moreover, since the regular superstructures are symmetric, it follows immediately from their definition:

$$\sigma_{-\mathbf{r}} = \sigma_{\mathbf{r}} \quad (\text{A I.2})$$

Then from (4) we get:

$$B(\mathbf{k}) = -\frac{1}{2} S \left\{ \sum_{\mathbf{r}} J_{\mathbf{r}} (1 - \sigma_{\mathbf{r}}) e^{i\mathbf{k}\mathbf{r}} + \sum_{\mathbf{r}} J_{-\mathbf{r}} (1 - \sigma_{-\mathbf{r}}) e^{-i\mathbf{k}\mathbf{r}} \right\} = -S \sum_{\mathbf{r}} J_{\mathbf{r}} (1 - \sigma_{\mathbf{r}}) \cos \mathbf{k}\mathbf{r} \quad (\text{A I.3})$$

which is a real function.

APPENDIX II

The identity of semiclassical and Ziman's results

The semiclassical treatment of spin waves in regular antiferromagnetic superstructures gives for isotropic exchange integrals (Cofta 1959):

$$E = \{[S(f_1 - \kappa) + \gamma \hbar H_A]^2 - S^2 f_2^2\}^{1/2} \quad (\text{A II.1})$$

where

$$\begin{aligned} f_1(\mathbf{k}) &= 2 \sum_{\mathbf{r}}^{+} J_{\mathbf{r}} (\cos \mathbf{k}\mathbf{r} - 1) \\ f_2(\mathbf{k}) &= 2 \sum_{\mathbf{r}}^{-} J_{\mathbf{r}} \cos \mathbf{k}\mathbf{r} \\ \kappa &= -2 \sum_{\mathbf{r}}^{-} J_{\mathbf{r}} \end{aligned} \quad (\text{A II.2})$$

and $\gamma < 0$ denotes the magnetomechanical ratio. The symbols \sum^{+} and \sum^{-} are used for the summation over the neighbours respectively parallel or antiparallel to the given spin (Such a notation is very useful for practical evaluation of sums over the neighbours). In the Ziman's notation, the sums (A II.2) may be written as:

$$\begin{aligned} f_1(\mathbf{k}) &= \sum_{\mathbf{r}} (1 + \sigma_{\mathbf{r}}) J_{\mathbf{r}} (\cos \mathbf{k}\mathbf{r} - 1) \\ f_2(\mathbf{k}) &= \sum_{\mathbf{r}} (1 - \sigma_{\mathbf{r}}) J_{\mathbf{r}} \cos \mathbf{k}\mathbf{r} \\ \kappa &= \sum_{\mathbf{r}} (\sigma_{\mathbf{r}} - 1) J_{\mathbf{r}} \end{aligned} \quad (\text{A II.3})$$

Considering that $\gamma \hbar = -g\beta$ and taking into account the formula (A I.3), we get:

$$S[f_1(\mathbf{k}) - \kappa] + \gamma \hbar H_A = -A(\mathbf{k}) \quad (\text{A II.4})$$

$$Sf_2(\mathbf{k}) = -B(\mathbf{k})$$

In this way the identity under consideration is demonstrated.

APPENDIX III

The power series expansion of the energy

In order to examine the validity of the expansion (10) let us consider first the natural superstructures of cubic lattices. According to the eq. (24) we are dealing in that case with a one variable only and the Taylor series has the form

$$E = \sqrt{C} \sum_{m=0}^{\infty} a_m k^m \quad (\text{A III.1})$$

where

$$a_m = \left(\frac{M}{C} \right)^{\frac{m}{2}} \cdot b_m$$

$$b_0 = 1$$

$$\left. \begin{aligned} b_{2n} &= -(-1)^n \frac{(2n-3)!!}{(2n)!!}, \\ b_{2n-1} &= 0 \end{aligned} \right\} n = 1, 2, 3, \dots$$

Let us determine the convergence radius k_r of (A III.1). By means of the well-known methods we get

$$k_r = \sqrt{\frac{|C|}{|M|}} \quad (\text{A. III.2})$$

From (29) we get

$$\left| \frac{C}{M} \right| = \frac{3\varepsilon_A}{S^2 |J_n z_n r_n^2 - J_s z_s r_s^2|} \quad (\text{A. III.3})$$

Only the order of magnitude of the k_r can be estimated, of course. We have to take into account that in the case of natural spin ordering, the exchange integral J_n must be inevitably the negative one. As to the integral J_s , a twofold situation can occur. Either $|J_s| \ll |J_n|$ and then the sign of the J_s is unimportant, or $|J_s| \sim |J_n|$ and then a simple examination of the semiclassical Hamiltonian leads to $J_s > 0$. In both the cases the denominator in (A III.3) is of the same order as $S^2 J_n^2 z_n^2 r_n^2$. Since for most antiferromagnetic substances holds (18), we can write:

$$\left| \frac{C}{M} \right| \sim \frac{3 \times 10^{-2}}{r_n^2} \quad (\text{A III.4})$$

Hence, we get

$$k_r \sim (6r_n)^{-1} \quad (\text{A III.5})$$

We have to examine also the question of validity of the approximation (10) i.e. of the neglecting of higher terms in the series (A III.1). The ratio

$$\left| \frac{a_1}{a_2} \right|, k^2$$

of absolute value of the third non-vanishing term to the second one is equal to

$$\frac{1}{4} \left| \frac{M}{C} \right| \cdot k^2$$

The third term may be ignored only if it amounts at most to a few percent of the second one. That implies the following requirement for the applicability of the approximation (10):

$$k^2 \lesssim \frac{1}{10} \left| \frac{C}{M} \right| = \frac{1}{10} k_r^2 \quad (\text{A III.6})$$

This inequality restricts the use of (10) rather more than the condition of convergence.

In the case of anisotropic superstructures the situation is a similar one, as can be seen from the formulas (34), (37), (42), (45) and (50), for a fixed direction. E.g. for *sc*-(001), making the assumption

$$\varepsilon_A \sim 2SB_0 \times 10^{-2}$$

analogous to (18), we obtain from (34):

$$\left| \frac{C}{M_{xx}} \right| \sim \frac{4 \times 10^{-2}}{a^2}$$

and (provided that $|J_n| \sim |J_s|$):

$$\left| \frac{C}{M_{xx}} \right| \sim \frac{3 \times 10^{-2}}{a^2}$$

Only if one of the exchange integrals J_n or J_s is equal to zero (extreme cases), the ratio $|C/M|$ may be sometimes 10^2 times larger than in (A III.4), at least for certain directions. So for transversal directions we find from (33) as well as from (36):

$$|M| = \frac{1}{4} a^2 |C|$$

for the second interactions term and from (43) we get the same equality for the nearest interactions term. From (40) we find $M^n = \frac{1}{8} a^2 |C|$ for the longitudinal direction. In (44) we get the same relation for the second interactions term for all directions. Nevertheless, all these examples do not remove our objections concerning the correctness of (10), because the cases of $J_n=0$ or $J_s=0$ in anisotropic superstructures seem impossible in practice. Consequently, the form (10) of the dispersion relation may be employed only for k being sufficiently small. The allowed values of k depend on $\varepsilon_A/2SB_0$. As follows from (A III.5) and (A III.6), k must fulfil the condition

$$ak \lesssim 10^{-2}$$

if the usual values $2SB_0 \sim \varepsilon_E$ are taken.

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LETTERS TO THE EDITOR

HÜCKEL'S THEORY: DEPENDENCE OF THE COULOMB INTEGRALS
ON THE ATOMIC CHARGES

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Formula (1) is assumed. ϵ is determined so as to yield the correct dipole moment for fulvene.

When applying Hückel's theory to alternant hydrocarbons, all core Coulomb integrals (α) are assumed equal. This assumption seems justified because all the carbon atoms bear equal charges (Coulson Longuet-Higgins 1947). For nonalternant hydrocarbons, however, the charge distribution is more complicated. Different carbon atoms bear different charges and, accordingly, the Coulomb integrals should be assumed different. No theory giving the dependence of the Coulomb integrals on the charges exists as yet. Wheland and Mann (1949), and Berthier and Pullman (1948, 1949), proposed $\alpha = q$, where q is the π -electronic charge on the carbon atom; their choice, however, was quite arbitrary (Pullman Pullman 1952). The only point that is clear is that α should be increased whenever the electronegativity of its carbon atom increases. If this is not done, the nonuniformity of the electronic distribution is overestimated. Thus, for instance, the conventional L.C.A.O. theory yields for the dipole moment of fulvene and azulene 4.8D and 6.4D (Debye units), respectively, whereas the experimental results are 1.2D and 1.0D (Pullman, Pullman 1952). Similar effects are to be expected for alternant hydrocarbons when ionized, as then electronic distribution is no longer uniform.

In this note the L.C.A.O. theory with selfconsistent values of both Coulomb (α) and resonance (β) integrals is used for computing the dipole moment of fulvene. The dependence of the core Coulomb integrals on the atomic charges is assumed similar to that proposed by Wheland and Mann:

$$\alpha = \epsilon q \quad (1)$$

where ϵ is a constant. It is our aim to find the value of ϵ yielding the correct dipole moment. The problem of whether formula (1) generalizes correctly Hückel's theory to nonalternant

hydrocarbons remains open, but were this the case indeed, the value of ε as found for fulvene should be generally applicable. The resonance integrals are assumed to depend on the lengths and orders of the bonds, according to the formula:

$$\beta = \beta_0 [1 - 2.683(R - 1.397 \text{ \AA}) + 3.599(R - 1.397 \text{ \AA})^2] \quad (2)$$

$$R - 1.397 \text{ \AA} = 0.180(\frac{2}{3} - p) \quad (3)$$

where p is the bond order, and R the bond length. The constants are those found by Coulson and Golebiewski (in print) using Longuet-Higgins and Salem's (1959) method. Usually an exponential formula was used instead of eq. (2), but the derivation (from the vibrational spectrum of benzene) gives no information on the terms beyond the quadratic one. Numerically the two formulae are equivalent if the accuracy does not exceed 0.001 \AA . Formula (2) is here preferred as yielding the force constant of ethylene more satisfactorily. (For the method of computation, see the paper by Longuet-Higgins and Salem).

The numerical results are given in Table 1, and the numbering of the atoms is shown in Fig. 1. Putting $\varepsilon=0$ and adjusting the resonance integrals, we reduce the dipole moment

Table 1.

	<i>a</i>	<i>b</i>	<i>c</i>
$R_{11'}$	1.424Å	1.441Å	1.445Å
$R_{21}=R_{2'1'}$	1.377Å	1.365Å	1.362Å
$R_{32}=R_{32'}$	1.436Å	1.450Å	1.454Å
R_{43}	1.381Å	1.365Å	1.361Å
$q_1=q_{1'}$	1.073	1.047	1.032
$q_3=q_{2'}$	1.092	1.054	1.044
q_3	1.047	1.035	0.991
q_4	0.622	0.762	0.857
μ	4.8D	3.0D	1.9D

a: Conventional L.C.A.O. theory.

b: L.C.A.O. theory with selfconsistent resonance integrals ($\varepsilon=0$).

c: L.C.A.O. theory with selfconsistent resonance and Coulomb integrals, $\varepsilon=1$.

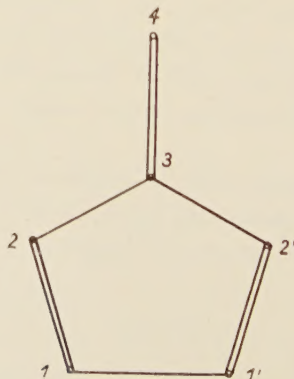


Fig. 1. Numbering of atoms in the fulvene molecule.

from 4.8D to 3.0D. This is only about 50% of the correction needed. As the next choice, ϵ was put equal to unity and the resulting L.C.A.O. equations were solved once more by the iterative method, starting with the best values of β obtained with $\epsilon=0$. The convergence was poor and the final result was obtained by an interpolation from the first four iterations (two overestimates and two underestimates of each charge). The resulting dipole moment, 1.9D, is still too large, which means that ϵ should exceed 1.

In order to estimate the right ϵ , two points were taken into consideration. Firstly, from the data compiled by Pullman and Pullman (1952), it appears that, for a wide variety of L.C.A.O. orbitals, the total dipole moment of fulvene is a smooth function of q_4 — the charge on the primary atom. On interpolating this function, it is found that the right value of the dipole moment (1.2D) corresponds to $q_4 \approx 0.928$. Secondly, the charges q_4 from the once iterated solutions for $\epsilon = 0$, $\epsilon = 0.7$, $\epsilon = 1.0$, and $\epsilon = 2.0$, when plotted as a function of ϵ , were found to lie very nearly on a straight line. Assuming that this linear dependence holds for further iterations also, we find from the results for $\epsilon = 0$ and $\epsilon = 1$ that the correct q_4 and, consequently, the correct dipole moment would be obtained for

$$\epsilon = 1.7 \quad (4)$$

Incidentally, it follows from the plot of q_4 versus ϵ that the iterative method diverges for values of ϵ greater than about 1.5.

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